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Ferro- and Antiferroelectric Substances

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II Data

Oxides

1 Perovskite-type oxides

1A Simple perovskite-type oxides

Nr. 1A-1 $NaNbO_3$, Sodium niobate

a	It was reported by MATTHIAS et al. in 1951 that $NaNbO_3$ was ferroelectric. CROSS et al., however, proved in 1955 that at room temperature it is not ferroelectric but antiferroelectric.	*51M2*, *55C2*
b	(see phase table below)	a) *61W2*, *58R3*

phase	V	IV	III*	II	I
state	F	A			P
crystal system	monoclinic	orthorhombic	pseudo-tetragonal	tetragonal	cubic
space group		Pbma a)-D_{2h}^{11}			Pm3m-O_h^1
Θ**	−200	354	562	640	°C

	$P_s \parallel [001]$ in phase V.	
	Phase IV: $a = 5.568$ Å ($\cong \sqrt{2} a_0$), $b = 5.505$ Å ($\cong \sqrt{2} a_0$), $c = 15.518$ Å ($\cong 4 a_0$), where a_0 is the lattice constant of the cubic cell of phase I.	*51V3*
	In phase IV (orthorhombic system) the longest edge of a unit cell is taken as the c axis (see Fig. 1). This system of the axes is adopted here. In Well and Megaw's analysis b and c axes were interchanged. The orthorhombic structure is also represented by a pseudomonoclinic unit cell (see Fig. 1), where $b' = c$, $a' = c'$ ($\cong a_0$), $\beta' \cong \pi/2$.	*61W2*
2a	Cooling method from a molten mixture of Na_2CO_3, Nb_2O_5, and NaF.	*51W1*
3	Crystal structure: In phase IV, $Z = 8$. Tab. 1; Fig. 1, 2.	
4	Lattice distortions (thermal expansion): For phase I, II, III, IV: Tab. 2,3; Fig. 3. For phase V, at −160 °C: $a = 5.564$ Å ($\cong \sqrt{2}\, a_0$), $b = 5.548$ Å ($\cong \sqrt{2}\, a_0$), $c = 7.812$ Å ($\cong 2\, a_0$), $\beta = 91°09'$. Fig. 4.	*57J1*
5a	Dielectric constants: Fig. 5. Curie-Weiss law: $\varkappa = C/(T - \Theta_p)$, $T > \Theta_{III-IV}$, where $C = 2 \cdots 4 \cdot 10^5$ °K and $\Theta_p = 60 \cdots 80$ °C.	*54S3*
c	Spontaneous polarization: $P_s \cong 12 \cdot 10^{-2}$ C m^{-2} ($\parallel c$, in phase V). Coercive and critical field for normal and double hysteresis curve: Fig. 6.	*55C2*
9a	Birefringence: Fig. 7, 8.	
14a	Domain structure: See	*55C2*, *64p1*, *62M9*, *62W3*
b	Dynamic properties: Fig. 9, 10.	

Tab. 1. $NaNbO_3$. Fractional coordinates x, y, z of atoms in unit cell at RT. [*61W2*]

	x	y	z
Na(1)	¾	0.250	0
Na(2)	0.769	0.251	¼
Nb	0.261	0.257	0.125
O(1)	¼	0.208	0
O(2)	0.271	0.290	¼
O(3)	0.010	0.532	0.121
O(4)	0.446	0.972	0.126

* According to Ismailzade phase III consists of 4 phases (see Fig. 3). [*63I4*]

** Transitions exhibit large temperature hysteresis, and the transition temperatures measured with decreasing temperature are given here.

Tab. 2. $NaNbO_3$. Lattice parameters at various temperatures. [*56F1*] and [*54S3*]

T [°C]	Crystal symmetry	Lattice parameters [*56F1*]	Lattice parameters [*54S3*]
20	Monoclinic	$a' = c' = 3.914$ Å $b' = 4 \cdot 3.881$ Å $\beta' = 90°\,39'$	$a' = c' = 3.915$ Å $b' = 4 \cdot 3.881$ Å $\beta' = 90°\,40'$
390	Pseudotetragonal	$a = 2 \cdot 3.920$ Å $c = 4 \cdot 3.926$ Å $c/a = 2.0032$	$a = 2 \cdot 3.919$ Å $c = 4 \cdot 3.927$ Å $c/a = 2.0040$
420	Pseudotetragonal	$a = 2 \cdot 3.924$ Å $c = 4 \cdot 3.924$ Å $c/a \approx 2.0000$	$a = 2 \cdot 3.921$ Å $c = 4 \cdot 3.927$ Å $c/a = 2.0028$
560	Tetragonal (changing to simple perovskite-type cell)	$a = 2 \cdot 3.933$ Å $c = 4 \cdot 3.940$ Å $c/a = 2.0038$	— — —
640	Cubic	$a = 3.942$ Å	—

Tab. 3. $NaNbO_3$. Lattice parameters of the subcell at various temperatures. [*63I4*]. See Fig. 3

T [°C]	Subcell parameters				
	pseudomonoclinic I ($a' = c' > b'$, $\beta' > 90°$)				
	a' [Å]	b' [Å]	β' −90°	a'/b'	V [Å³]
18 ··· 20	3.914_7	3.885	40'	1.0075_5	59.5_3
100	3.917	3.893_6	37	1.0060	59.7_4
150	3.919_5	3.898_7	33	1.0055	59.9
200	3.922_4	3.902_6	29	1.0050	60.0_5
250	3.924_3	3.907_5	26	1.0040	60.1_7
300	3.925_6	3.914	22	1.0030	60.3_2
340	3.926_3	3.917_5	18	1.0025	60.4
350	3.926_5	3.919	17	1.0020_2	60.4_2
	pseudomonoclinic II				
360	3.927_2	3.920	6	1.0020	60.45
380	3.927_8	3.921_3	5	1.0015_9	60.50
400	3.928_3	3.922_3	4	1.0015	60.5_2
	pseudomonoclinic III				
420	3.929_4	3.923	3	1.0015	60.5_5
440	3.930	3.924	3	1.0015	60.60
460	3.932	3.926_3	3	1.0015	60.70
	pseudomonoclinic IV				
480	3.933_5	3.927_5	3	1.0015_3	60.7_7
500	3.934_5	3.928_8	2	1.0015	60.8_2
510	3.935	3.929_5	2	1.0015	60.85

tetragonal I

T [°C]	c [Å]	$a = b$ [Å]	c/a	V [Å³]
520	3.936_7	3.929_5	1.0015_9	60.80
540	3.938	3.930_2	1.0020	60.85
560	3.939_8	3.931_6	1.0020_8	60.90
	tetragonal II			
580	3.941_4	3.934_2	1.0020	61.00
600	3.943_4	3.937_8	1.0015	61.15
620	3.945_6	3.942	1.0010	61.30
630	3.945	≈3.945	≈1.0000	61.40

cubic

T [°C]	a_0 [Å]	V [Å³]	T [°C]	a_0 [Å]	V [Å³]
640	3.947_3	61.50	700	3.949_7	61.6_2
650	3.947_6	61.5_2	720	3.950_6	61.6_7
680	3.949	61.5_7			

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Nr. 1A-2 $KNbO_3$, Potassium niobate

		Ref.
1a	Ferroelectricity in $KNbO_3$ was first discovered by MATTHIAS in 1949.	49M4
b	phase: IV / III / II / I state: F / F / F / P crystal system: rhombohedral / orthorhombic / tetragonal / cubic space group: — / Bmm2[a])-C_{2v}^{14} / — / Pm3m-O_h^1 Θ: −10 / 225 / 435 °C	[a])63K2
	$P_s \parallel [001]$ in phase II (along [001] of phase I), $P_s \parallel [001]$ in phase III (along [110] of phase I), $P_s \parallel [111]$ in phase IV (along [111] of phase I). $T_{melt} = 1050$ °C $\varrho = 4.590 \cdot 10^3$ kg m^{-3} $a = 5.697$ Å, $b = 3.971$ Å, $c = 5.720$ Å at RT. Transparent. Light yellow.	 55R3, 58M3 52L1 67K4
2	Flux method (K_2CO_3 flux). Phase diagram of K_2CO_3-Nb_2O_5 system; see Pulling method from the K_2CO_3-Nb_2O_5 mixture Crystal form: square plate	51W1 55R3 58M3
3	Crystal structure: $Z = 1$ in phase I, II, IV. $Z = 2$ in phase III. Tab. 4, 5; Fig. 11.	
4	Temperature dependence of lattice parameters: Tab. 6; Fig. 12.	
5	Dielectric constant: Fig. 13, 14. $\varkappa = C/(T - \Theta_p)$, $T > \Theta_{II-I}$, where $C = 2.42 \cdot 10^5$ °K, $\Theta_p = 360$ °C. Nonlinear dielectric properties: $\xi = -1.62 \cdot 10^9$ J C^{-4} m^5, $\zeta = 1.79 \cdot 10^{10}$ J C^{-6} m^9. Spontaneous polarization and coercive field: Fig. 15. $P_s = 26 \cdot 10^{-2}$ C m^{-2} at $T = \Theta_p$.	 56T3 56T3 56T3
6	Transition heat, transition entropy: Tab. 7.	56T3
7	Piezoelectricity: Fig. 16.	
12	NQR: Tab. 8; Fig. 17 ⋯ 20.	

Tab. 4. $KNbO_3$. Atomic positions in fractional coordinates at RT in phase III. [67K4]

Nb	0, 0, 0
K	$0, \frac{1}{2}, \frac{1}{2} + z_K$
O(1)	$0, \frac{1}{2}, z_1$
O(2)	$\frac{1}{4} + x_2, 0, \frac{1}{4} + z_2$
z_K	+0.017
z_1	+0.021
z_2	+0.035
x_2	+0.004

Tab. 5. $KNbO_3$. Interatomic distances and bond angles at RT. [67K4]

	*	distance Å	**	*	angle °
Nb-O(1)	(2)	1.991 ± 0.001	O(2)(*s*)-Nb-O(2)(*s*)	(1)	97.4 ± 1.2
Nb-O(2)	(2)	1.863 ± 0.007	O(2)(*l*)-Nb-O(2)(*l*)	(1)	83.4 ± 1.0
Nb-O(2)	(2)	2.180 ± 0.009	O(2)(*s*)-Nb-O(2)(*l*)	(2)	89.7 ± 0.5
K-O(1)	(1)	2.837 ± 0.014	O(1)-Nb-O(2)(*s*)	(4)	92.3 ± 0.6
K-O(1)	(2)	2.848 ± 0.001	O(1)-Nb-O(2)(*l*)	(4)	87.5 ± 0.6
K-O(1)	(1)	2.883 ± 0.014	Nb-O(1)-Nb	(1)	172.8 ± 0.7
K-O(2)	(4)	2.792 ± 0.008	Nb-O(2)-Nb	(2)	168.6 ± 0.6
K-O(2)	(4)	2.873 ± 0.010			
O(1)-O(2)	(4)	2.780 ± 0.012			
O(1)-O(2)	(4)	2.884 ± 0.012			
O(2)-O(2)	(1)	2.802 ± 0.024			
O(2)-O(2)	(1)	2.894 ± 0.024			
O(2)-O(2)	(2)	2.860 ± 0.001			

* Numbers in this column indicate numbers of equal bonds or angles per formula unit.
** For the O-Nb-O angles, the letter *s* or *l* indicates whether the Nb-O(2) bond involved is short or long.

Tab. 6. $KNbO_3$. Lattice constants and volume of unit cell at various temperatures. [54S3]. a', c': lattice parameters of pseudotetragonal cell

T °C	$a' = c'$ Å	b Å	b/a	β	V Å^3
25	4.0375	3.9711	1.0167	90° 15'	64.73
125	4.0374	3.9797	1.0145	90° 15'	64.87
185	4.0363	3.9830	1.0134	90° 13'	64.89
205	4.0369	3.9839	1.0133	90° 14'	64.93
	$a = b$	c	c/a		
220	3.9972	4.0636	1.0166		64.92
230	3.9978	4.0640	1.0166		64.95
270	3.9992	4.0647	1.0164		65.01
320	4.0023	4.0639	1.0154		65.10
375	4.0048	4.0620	1.0143		65.15
410	4.0080	4.0567	1.0122		65.18
425	4.0214				65.03
450	4.0225				65.09
510	4.0252				65.22

Tab. 7. $KNbO_3$. Transition heat and transition entropy per mole. [54S1]

Transition	ΔQ_m cal mol^{-1}	ΔS_m cal °K^{-1} mol^{-1}
IV → III	32	0.12
III → II	85	0.17
II → I	190	0.28
	134	—

Tab. 8. $KNbO_3$. NQR spectrum. [54C1]. The measured frequency ratios intersect the calculated ratios in a straight line at constant $\eta = 0.806 \pm 0.002$. η = asymmetry parameter

Crystal structure	f MHz	Measured ratio	Calculated ratio ($\eta = 0.806$)	Identification	e^2qQ/h MHz
orthorhombic (20 °C)	3.648				
		1.204	1.204	(9/2, 7/2)	23.120 ± 0.05
	3.030				
		1.198	1.196	(3/2, 1/2)	
	2.527				
		1.214	1.213	(7/2, 5/2)	
	2.085			(5/2, 3/2)	
rhombohedral (−196 °C)			($\eta = 0.0$)		
	2.674				
		1.335	1.333	(9/2, 7/2)	16.0 ± 0.1
	2.004				
		1.503	1.500	(7/2, 5/2)	
	1.335			(5/2, 3/2)	

Nr. 1A-3 $NaTaO_3$, Sodium tantalate

1a It was reported by MATTHIAS in 1949 that $NaTaO_3$ is ferroelectric below 480 °C. No anomalies of the dielectric constants, however, were observed by SMOLENSKII et al. 49M1, 57S3

b

phase	IV	III	II	I	
state	(F)				
crystal system	orthorhombic	orthorhombic	tetragonal	cubic	
space group	$Pc2_1n\text{-}C_{2v}^9$				57K1
Θ	480	550	630	°C	57K1

$a = 5.4941$ Å, $b = 7.7508$ Å, $c = 5.5130$ Å at RT. 62I4

The cubic cell in phase I becomes pseudomonoclinic in phase IV. Relation between the orthorhombic unit cell and the pseudomonoclinic cell: Fig. 21. 51V2

3 Crystal structure: $Z = 4$.
Atomic positions: Tab. 9; Fig. 22.

4 Temperature dependence of lattice parameters: Tab. 10; Fig. 23.

Tab. 9. $NaTaO_3$. Fractional coordinates of atoms in the unit cell. [57K1]

Na	x:	$0 - 0.01$	$0 + 0.01$	$\frac{1}{2} - 0.01$	$\frac{1}{2} + 0.01$
	y:	$\frac{3}{4} + 0.03$	$\frac{1}{4} + 0.03$	$\frac{1}{4} + 0.03$	$\frac{3}{4} + 0.03$
	z:	$0 + 0.02$	$0 - 0.02$	$\frac{1}{2} - 0.02$	$\frac{1}{2} + 0.02$
Ta*	x:	$\frac{1}{2}$	$\frac{1}{2}$	0	0
	y:	0	$\frac{1}{2}$	$\frac{1}{2}$	0
	z:	0	0	$\frac{1}{2}$	$\frac{1}{2}$
O(1)	x:	$0 - 0.02$	$0 + 0.02$	$\frac{1}{2} + 0.02$	$\frac{1}{2} - 0.02$
	y:	$\frac{3}{4} + 0.01$	$\frac{1}{4} + 0.01$	$\frac{3}{4} + 0.01$	$\frac{1}{4} + 0.01$
	z:	$\frac{1}{2} + 0.02$	$\frac{1}{2} - 0.02$	$0 + 0.02$	$0 - 0.02$
O(2)	x:	$\frac{1}{4} + 0.04$	$\frac{1}{4} - 0.04$	$\frac{3}{4} - 0.04$	$\frac{3}{4} + 0.04$
	y:	$0 - 0.03$	$0 - 0.03$	$\frac{1}{2} - 0.03$	$\frac{1}{2} - 0.03$
	z:	$\frac{1}{4} + 0.04$	$\frac{3}{4} + 0.04$	$\frac{3}{4} - 0.04$	$\frac{1}{4} - 0.04$
O(3)	x:	$\frac{1}{4} + 0.04$	$\frac{1}{4} - 0.04$	$\frac{3}{4} - 0.04$	$\frac{3}{4} + 0.04$
	y:	$\frac{1}{2} + 0.06$	$\frac{1}{2} + 0.06$	$0 + 0.06$	$0 + 0.06$
	z:	$\frac{1}{4} + 0.04$	$\frac{3}{4} + 0.04$	$\frac{3}{4} - 0.04$	$\frac{1}{4} - 0.04$

Tab. 10. $NaTaO_3$. Temperature dependence of the pseudo-cell parameters. [62I4]. For the notations, see Fig. 21

T [°C]	23	100	200	300	400	450	480	500	550	580	600
$a' = c'$ [Å]	3.889_5	3.893_6	3.899_5	3.907	3.912_8	3.916	3.918	3.920	3.923	3.925_2	3.927
b' [Å]	3.885_5	3.890_5	3.896_5	3.903_8	3.910_2	3.913_6	3.915_8	3.918	3.923	$\approx 3.925_2$	≈ 3.927
$\beta - 90°$	22'00"	16'00"	9'00"	6'00"	4'00"	3'30"	2'00"	≈2'00"	1'30"	0'00"	0'00"
a'/b'	1.0010	1.0009	1.0009	1.0008	1.0006	1.0006	1.0005	1.0005	1.000	1.000	1.000
V [Å³]	58.8_0	59.0_0	59.2_5	59.5_5	59.8_5	60.0_0	60.1_0	60.2_0	60.3_5	60.4_5	60.5_5

T [°C]	630	660	680
$b = a = c$ [Å]	3.929	3.931	3.932_5
V [Å³]	60.6_5	60.7_5	60.8_0

Nr. 1A-4 $KTaO_3$, Potassium tantalate

1a	Ferroelectric activity was first reported by MATTHIAS in 1949;[a]) however, recent studies by WEMPLE have proved that the ferroelectric transition does not occur, at least above 1.6 °K.[b])	[a]) *49M1, 49M4* [b]) *64W2, 65W2*
b	$KTaO_3$ is cubic and its space group is Pm3m-O_h^1.	*64W2, 65W2, 51V2*
	$T_{melt} = (1357 \pm 3)$ °C.	*55R2, 56R2*
	$\varrho = 6.97 \cdot 10^3$ kg m^{-3}.	*58R1*
	$a = 3.9885$ Å at RT.	*51V2*
	Transparent, colorless or pale blue (blue in oxygen-deficient crystals).	*64W2*
	Cleavage: along (100) planes.	
	Hardness: nearly the same as quartz.	
2a	Flux method: KF flux,[a]) dark small crystals; K_2CO_3 flux,[b]) large (≈10 mm) transparent crystals.	[a]) *62T5, 64W2* [b]) *66U1*
	Czochralski-Kyropoulos method: large (≈10 mm) good quality crystals.	*64W2, 65W2, 67B7*
	Floating technique: planar single crystals.	*66W8*
	Phase diagram of system K_2CO_3-Ta_2O_5: Fig. 24.	
	Hydrothermal phase diagram K_2O-Ta_2O_5-H_2O at 400 °C:	*67M2*
3	$Z = 1$ Crystal structure: cubic perovskite type, (Pm3m-O_h^1). K at 1a position; Ta at 1b position; 3O at 3c position.	*51V1, 51V2*

* All positions ±0.002.

	Nr. 1A-4 $KTaO_3$ continued	
4	$a = 3.9885$ Å at RT; $a = 4.0026$ Å at 450 °C.	51V2, 59B1
5a	Dielectric constant at low frequencies: earlier studies showed a peak in the $\varkappa$ vs. T curve;[a]) recent measurements have shown that no peak exists down to 1.6 °K.[b]) Fig. 25. $\varkappa = 243$ at RT. $\varkappa = \varkappa_0 + C/(T - \Theta_p)$ $T > 30$ °K, where $\varkappa_0 = 48$, $C = 5.7 \cdot 10^4$ °K, $\Theta_p = 4$ °K. Loss tangent: $\tan\delta \approx 0.001$ at 200 kHz at RT. Dielectric constant in the GHz range: Fig. 26. Q values in the GHz range: $Q = 10^3 \cdots 10^4$. Dielectric loss in the far infrared frequency range: See 1A-4-9 below (Figs. 34, 35). Hydrostatic pressure dependence of the reciprocal dielectric constant: Fig. 27.	a)50H3 b)65W2, 64W2 65W2 64W2 64R3 64W2
b	Effects of dc bais on $\varkappa$ at 4.2 °K and at RT: Figs. 28, 29. Coefficients in free energy expansion: $\xi = 9 \cdot 10^9$ V m^5 C^{-3} at 4.2 °K, $\xi = (4 \pm 1) \cdot 10^9$ V m^5 C^{-3} at 295 °K.	65K1 65W2
c	D vs. E curves show no hysteresis character down to 1.6 °K. P vs. E at 4.2 °K: see	64W2
9a	Refractive index in visible region: Fig. 30. Reflectivity in far infrared region and the dispersion: Figs. 31, 32. Reflectivity data were used to obtain transverse optical modes of the lattice vibration by means of Kramers-Kronig relation (cf. Tab. 42). Transverse optical modes as a function of temperature: Tab. 11; Fig. 33. The square of the wave number $\tilde{\nu}_{t1}$ for the "ferroelectric mode" is approximately linear to T: $\tilde{\nu}_{t1}^2 \propto (T - \Theta_p)$ (Additional data are given on the ferroelectric soft mode, see 1A-4-13b). (Additional data are given on the fluorescent spectrum of Eu^{3+} in $KTaO_3$: see Effect of lattice vibration on the fluorescent spectrum and the conductivity in the far infrared Imaginary part of the dielectric constant and the conductivity in the far infrared region: Figs. 34, 35. Absorption coefficient α depends on the degree of oxygen reduction in $KTaO_3$. Absorption coefficient near the interband absorption edge (about 3.6 eV) for insulating and semiconducting $KTaO_3$: Fig. 36 (for additional data, see Fig. 2 of reference). Absorption vs. wavelength of light: Fig. 37. Absorption vs. carrier concentration in semiconducting $KTaO_3$: Fig. 38. Optical absorption in impurity doped single crystals: for impurities Fe, Mn, Co and Cr, see	63M4, 67P4 67P4, 67F2 65S9 65W2 67B1 64W2
b	Quadratic electrooptic constants (6328 Å, 2 ⋯ 77 °K): $M_{11} - M_{12} = (0.16 \pm 0.01)$m^4 C^{-2}; $M_{44} = (0.12 \pm 0.01)$ m^4 C^{-2}. Electroreflectance and electroabsorption were studied using semiconducting $KTaO_3$. Effect of interface dc field on the reflectance of the (100) surface: Fig. 39. Electroreflectance spectra of (100) and (111) surfaces: Figs. 40, 41. Effect of polarization of light on the electroreflectance: Fig. 42. Electroreflectance as a function of the surface polarization: Fig. 43. Electroreflectance singularities and the corresponding energies: Tab. 12. Electroabsorption near the absorption edge: Fig. 44. Fundamental absorption edge (≈ 3.6 eV) shifts to higher energies with dc bias: Fig. 45.	64G3, 63G3 67F4 67B1, 66B2
d	Faraday rotation near the band edge: Fig. 46; Tab. 44.	67F2
f	Electric-field-induced Raman effect: Fig. 47. (For the ferroelectric soft mode obtained from the Raman scattering, see Fig. 33). Fluorescence spectrum of Eu^{3+} in $KTaO_3$: see	65S9 65W2
10	Resistivity of insulating single crystal: $\varrho > 10^8$ Ωm at RT. Most data on the transport properties have been obtained using oxygen-deficient semiconducting $KTaO_3$. Resistivity of oxygen-deficient single crystals as a function of temperature: Fig. 48. Resistivity of oxygen-deficient single crystals at RT (see also Tab. 13). Hall mobility: $\mu_H = 3 \cdot 10^{-3}$ m^2 V^{-1} sec^{-1} at RT; Fig. 49. $\mu_H \approx 8 \cdot 10^4$ T^{-3} m^2 V^{-1} sec^{-1}, $T > 100$ °K; Fig. 49. Hall coefficient and Hall mobility at 4.2 °K and RT for several semiconducting $KTaO_3$: Tab. 13. Hall mobility vs. carrier concentration: Fig. 50. Scattering cross section vs. carrier concentration: see Ca concentration in doped $KTaO_3$ vs. net ionized donor concentration: see Electrical conductivity vs. hydrostatic pressure: Fig. 51. Conductivity in the far infrared region: see Fig. 35. Seebeck coefficient: $Q = 550$ μV °K^{-1} at RT. (Oxygen-deficient $KTaO_3$ with $N = 3.5 \cdot 10^{23}$ m^{-3}). Effective mass estimated from the Seebeck coefficient: $m^* = (0.8 \pm 0.28)\, m_0$. Photoconductivity vs. $h\nu$ shows a peak at $h\nu = 3.58$ eV.	65W2 65W2 66S17 66W5 65W2 65W2 65W2

12a NMR of ^{181}Ta in $KTaO_3$: spin-lattice relaxation time, $T_1 \approx 10^{-3}$ sec at RT; spin-spin relaxation time, $T_2 = \approx 10^{-5}$ sec at RT; nuclear magnetic moment of ^{181}Ta ($I = 7/2$): $p_n = (2.340 \pm 0.001)\ \mu_n$ (uncorrected); ($p_n = (2.35 \pm 0.01)\ \mu_n$, after estimated corrections). — *60B2*

Nuclear magnetic acoustic resonance: the absorption data were given for $\Delta m = \pm 2$ transition of ^{181}Ta as a function of the angle between magnetic field and sound axis [100]. — *67M4*

b ESR of Eu^{2+} and Gd^{3+} in $KTaO_3$: Tab. 14. — *66U1*
ESR of Fe^{3+}: $g = 1.99 \pm 0.01$; $|a| = (345 \pm 10) \cdot 10^{-2}\ m^{-1}$ at 4.2 °K; — *64W2*
$a = (288 \pm 5) \cdot 10^{-2}\ m^{-1}$ at RT (Fe^{3+} is on the Ta^{5+} site). — *67H3*
$a = (30 \pm 1) \cdot 10^{-2}\ m^{-1}$ at RT (Fe^{3+} is on the K^{1+} site). — *67H3*
ESR Stark effect for Fe^{3+}: E_{bias} along [100] induces axial splitting term D ($D = 12 \cdot 10^{-2}\ m^{-1}$ at $E_{bias} = 1.0$ MV m^{-1} at 4.2 °K; $D \propto E^2_{bias}$). — *63W5, 64W2*
ESR of Ni^{3+} located on Ta^{5+} site (low spin state) and on K^{1+} site: see — *67H3, 65H2*
ESR in Mn-doped, Co-doped and Cr-doped $KTaO_3$: see — *64W2*

13b Phonon dispersion relation for the transverse optical branch: Fig. 52; Tab. 15. — *67S11*
Temperature dependence of the ferroelectric soft mode: Fig. 53.
The square of the phonon energy of the ferroelectric soft mode can be approximated by $(h\nu)^2 = 10^4\ A/\varkappa$, 40 °K < T < 295 °K; where $A = 2.825\ (\text{meV})^2$, $\varkappa(T)$ is the dielectric constant. — *67S11*
For the ferroelectric soft mode, see also 1A-4-9a.
Phonon energies of the acoustic modes: Fig. 54.

17 Etchant: single crystal is slowly etched by dilute HF. — *64W2*
Band structure and the related properties: see references; also 1A-4-9a, 9b, 9d, 10, and Tab. 12. — *67F4, 67B1*
Band gap energies determined by various methods:

Method	296 °K	77 °K
Faraday rotation	3.77 eV 3.62 eV	3.79 eV 3.65 eV
Electroreflectance singularities	3.57 eV 3.80 eV	
Absorption data Energy at which $\alpha \approx 10^6\ m^{-1}$	3.75 eV 3.79 eV	

67B1

Cyclotron resonance of semiconducting $KTaO_3$ at 70 GHz and 1.4 °K: microwave skin depth, about 30 μm; see reference paper for the microwave absorption vs. magnetic field curves. — *65S13*

Tab. 11. $KTaO_3$. Transverse optical modes at various temperatures [*67P4*]. The wave number $\tilde{\nu}_{t1}$ (ferroelectric soft mode) is temperature dependent.

T [°K]	$\tilde{\nu}_{t1}$	$\tilde{\nu}_{t2}$	$\tilde{\nu}_{t3}$
	$\cdot 10^2\ m^{-1}$		
12	25	196	—
126	58	198	551
232	79	198	551
295	88	199	550
463	106	199	—

Tab. 12. $KTaO_3$. (Ca-doped). Singularities observed in electroreflectance spectra (in eV) [*67F4*]. See Figs. 40, 41

	E_1	E_2	A_1	A_1'	A_2
	[eV]				
$KTaO_3$ (100)	3.57	3.80	4.40	4.88	5.50
$KTaO_3$ (111)	—	3.77	4.45	4.90	5.47
$KTaO_3$ (110)	3.55	3.80	4.47	4.85	5.50

Tab. 13. $KTaO_3$ (reduced). Hall coefficient R_H and Hall mobility μ_H at 295 °K and 4.2 °K for single crystals [*65W2*]. Carrier concentrations N are calculated from the 4.2 °K Hall coefficient using $R_H = -1/Ne$

Sample Nr.	N_{calc} m^{-3}	R_H $m^3\ C^{-1}$ (295°K)	R_H $m^3\ C^{-1}$ (4.2°K)	μ_H $m^2\ V^{-1}\ sec^{-1}$ (295°K)	μ_H $m^2\ V^{-1}\ sec^{-1}$ (4.2°K)
1	$3.5 \cdot 10^{23}$	$20.3 \cdot 10^{-6}$	$18 \cdot 10^{-6}$	$2.7 \cdot 10^{-3}$	2.3
2	$6.0 \cdot 10^{23}$	$12.9 \cdot 10^{-6}$	$10.4 \cdot 10^{-6}$	$2.9 \cdot 10^{-3}$	1.9
3	$6.6 \cdot 10^{23}$	$11.5 \cdot 10^{-6}$	$9.4 \cdot 10^{-6}$	$3.1 \cdot 10^{-3}$	1.9
4	$2.4 \cdot 10^{24}$	$3.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	1.1
5	$7.8 \cdot 10^{24}$	$1.0 \cdot 10^{-6}$	$0.80 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	0.53
6	$1.3 \cdot 10^{25}$	$0.62 \cdot 10^{-6}$	$0.48 \cdot 10^{-6}$	$3.1 \cdot 10^{-3}$	0.34

Tab. 14. $KTaO_3$. Parameters of ESR spectrum of Eu^{2+} and Gd^{3+} ions, doped in single crystals of $KTaO_3$ [*66U1*]

Para-magnetic center	Site	S	$\mathcal{H}$	ν GHz	T °K	g-factor	FS b_{40}, b_{60} 10^{-2} m^{-1}	HFS I	HFS A 10^{-2} m^{-1}
Eu^{2+}	K^+	7/2	(8)	9.1	77	1.990 ± 0.002	$b_{40} = (\pm)16 \pm 2$ $b_{60} = (\pm)1.2 \pm 0.6$	5/2 5/2	$\|^{151}A\| = 36 \pm 1$ $\|^{153}A\| = 16 \pm 1$
Gd^{3+}		7/2			4.2	1.990 ± 0.002	$b_{40} = -8.14 \pm 0.27$ $b_{60} = +0.47 \pm 0.3$		
					77	1.990 ± 0.002	$b_{40} = -7.0 \pm 0.3$ $b_{60} = +0.5 \pm 0.5$		

Tab. 15. $KTaO_3$. Phonon energies of the soft ferroelectric mode (transverse optical mode) at various temperatures [*67S11*]. The wave vector q at the zone boundary is 0.788 Å^{-1} ($= \pi/a$). See Fig. 52

T °K	Phonon energy [meV] for q [Å^{-1}] = 0	0.1	0.2
295	10.7	11.5	13.5
230	9.7		
170	8.6	10.0	12.5
120	7.3		
77	5.7	7.5	10.7
40	4.2	6.0	
28	3.6	5.9	10.5
15	3.0	5.3	
10	3.2	5.2	
4	3.1	5.3	9.8

Nr. 1A-5 $CaTiO_3$, Calcium titanate (Perovskite)

Tab. 16. $CaTiO_3$. Ion positions. [*57K2*]

4 Ti in 4(a):	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2};\ \frac{1}{2}, \frac{1}{2}, 0;\ 0, \frac{1}{2}, \frac{1}{2}$.
4 Ca in 4(c):	$x, \frac{1}{4}, z;\ \bar{x}, \frac{3}{4}, \bar{z};\ \frac{1}{2}+x, \frac{3}{4}, \frac{1}{2}-z;\ \frac{1}{2}-x, \frac{1}{4}, \frac{1}{2}+z;$ with $x = 0$, $z = 0.030$.
4 O in 4(c):	with $x = \frac{1}{2} - 0.037$, $z = -0.018$.
8 O in 8(d):	$x, y, z;\ \frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}+z;$ $\bar{x}, \frac{1}{2}+y, \bar{z};\ \frac{1}{2}+x, \bar{y}, \frac{1}{2}-z;$ $\bar{x}, \bar{y}, \bar{z};\ \frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}-z;$ $x, \frac{1}{2}-y, z;\ \frac{1}{2}-x, y, \frac{1}{2}+z;$ with $x = \frac{1}{4} - 0.018$, $y = -0.026$, $z = \frac{1}{4} - 0.018$.

1a Specific heat anomaly associated with a phase transition was observed in $CaTiO_3$ at about 1260 °C by Naylor et al. in 1946. Gränicher et al. reported that $CaTiO_3$ becomes cubic above 1260 °C. *46N1, 54G1*

b

phase	II	I	
state		P	*54G1*
crystal system	orthorhombic	cubic	*57K2*
space group	Pcmn-D_{2h}^{16}		*46N1*
Θ	≈1260 °C		*62M3*

$\varrho = 4.10 \cdot 10^3$ kg m^{-3} at RT. *62M3*
$T_{melt} = 1960$ °C *57K2*
$a = 5.3670$ Å, $b = 7.6438$ Å, $c = 5.4439$ Å at RT.
The ideal perovskite cubic unit cell becomes pseudo-monoclinic in phase II in the same manner as shown in Fig. 21. $\beta' = 90° 48'$ at RT.
Transparent, colorless. *57K2*

2 Flux method; flux: $CaCl_2$, $BaCl_2$, $CaCl_2+BaCl_2$, $Na_2CO_3+K_2CO_3$. *58L1, 62M3*
Flame fusion method: *57K2*

3 Crystal structure: $Z = 4$ in phase II.
Fig. 55; Tab. 16.

4 Lattice distortion: Fig. 56. *62M3*

5a Dielectric constant: $\varkappa = 186$, $\tan\delta = 3 \cdot 10^{-4}$ at RT.
Fig. 57.

6a Specific heat: Fig. 58. *46N1*
Transition heat: $\Delta Q = 550$ cal mol^{-1} at Θ_{II-I}.

	Nr. 1A-5 $CaTiO_3$ continued	
9a	Refractive indices: Fig. 59. Reflection and absorption: Fig. 60, 61.	
17	Hardness: Mohs 6.5 ··· 7, Knoop 986	*62M3*

Nr. 1A-6 $SrTiO_3$, Strontium titanate

1a	Ferroelectric-like behavior of $SrTiO_3$ was first observed by GRÄNICHER in 1956.	*56G2*
b	(phase data, see table below)	*62R1*

phase	II*	I
state	(F)	P
crystal system	tetragonal	cubic**
space group		Pm3m-O_h^1
Θ	110	°K

	$T_{melt} \cong 2000$ °C. $\varrho = 5.11 \cdot 10^3$ kg m^{-3}. $a = 3.905$ Å at RT. Transparent, colorless	*63f2, 64l1* *63f2* *64L4*
2a	Crystal growth: Flux method (flux: KF or 50% Na_2CO_3 + 50% K_2CO_3). Flame-fusion (Verneuil) method. Phase diagram of the system SrO-TiO_2 is given in Figs. 297 and 289 of [*64l1*].	*57N1* *61G1* *64l1*
3	Crystal structure: $Z = 1$. Fig. 62.	
4	Thermal expansion: Fig. 63.	
5a	Dielectric constant: Figs. 64 ··· 76. Expression of $\varkappa$ vs. T curve: Curie-Weiss law: $\varkappa = C/(T - \Theta_p)$, $T > 70$ °K, where $C = 7.83 \cdot 10^4$ °K, $\Theta_p = 28$ °K $\varkappa = M/[(T_1/2)\coth(T_1/2T) - T_0]$, $T < 50$ °K, where $T_0 = 38$ °K, $T_1 = 84$ °K, $M = 9 \cdot 10^4$ °K.	 *61M3* *59W2, 62S2*
b	Coefficients of free energy expansion at low temperatures:	*66C6*
c	Saturation polarization: Fig. 77. Remanent polarization: Fig. 78.	
d	Electrocaloric effect: Fig. 79. For additional data, see	 *64K5, 65H4, 61H1*
6a	Specific heat: Fig. 80. Specific heat below 1 °K, see	 *61g1, 66A4*
b	Thermal conductivity: Figs. 81, 82. For ceramics: see also	 *58Y1, 60Y1, 61g1, 66H9*
7a	Piezoelectricity (dc bias induced piezoelectricity): Figs. 83, 84, 85.	
b	Electrostriction: Fig. 86.	
8a	Elastic compliances and stiffnesses: Tab. 17; Figs. 87, 88, 89.	
9a	Refractive indices: Tabs. 18, 19; Fig. 90. Reflectivity, absorption coefficient and dielectric constant: (i) Infrared region: Figs. 91 ··· 95. See also Tab. 42. (ii) Visible and ultraviolet region: Figs. 96 ··· 102. See also Tab. 43.	
b	Quadratic electrooptic effect: $M_{11} - M_{12} = (0.14 \pm 0.01)$ m^4 C^{-2} at 6328 Å (4.2 ··· 300 °K).	*64G3*
c	Piezooptic effect: Tabs. 20, 21.	

* In phase II a hysteresis loop is observed,[a]), [b]) but the remanent polarization depends upon the amplitude of the applied field. According to LYTLE, phase II consists of three phases. [a]) [*59W2*], [b]) [*61M3*], [*64L4*]

** Generally the phase I is believed to be cubic but evidence of pseudo-cubic structure was reported by a few authors. [*64L4*], [*66C6*]

	Nr. 1A-6 $SrTiO_3$ continued	
9d	Faraday rotation: Fig. 103. See also Tab. 44.	67B1
e	Raman effect: Fig. 104.	66K1
	Brillouin scattering: Fig. 105. See	61g1
10	Electrical resistivity: $\varrho > 10^7\ \Omega$m (good quality single crystal) at RT. Fig. 106. For additional data, see Tab. 22.	61g1
	Resistivity, Hall coefficient and Hall mobility of semiconductive samples: Tab. 23; Figs. 107 ··· 110. For additional data, see	64F5, 67T6
	Hall mobility for photo-excited electron: see Fig. 115.	66T10
	Piezoresistivity: Figs. 111, 112, 113.	
	Photoconductivity: Figs. 114, 115.	
	Photoemission: Fig. 116.	64S5
	Superconductivity: discovered in semiconductive $SrTiO_3$ by Schooley et al. in 1964. Figs. 117 ··· 120. Tab. 24.	
	Penetration depth of static magnetic field in superconductive $SrTiO_3$ is of the order of 10^{-5} m.	66S16
11	Magnetic susceptibility: Tab. 25.	
12a	NMR: Fig. 121.	
b	ESR: Tab. 26; Figs. 122 ··· 130.	
c	Mössbauer effect: Figs. 131, 132.	
13c	Inelastic neutron scattering: Tab. 27; Figs. 133, 134, 135.	
14a	Domain structure: A fine twin structure was observed in phase II. The appearance of the twin structure is similar to that of the 90° domains in tetragonal $BaTiO_3$. The dc field, however, does not change the twin structure.	61M3, 64L4
16	Radiation damage: Fig. 136.	66R6
17	Etching and chemical polishing:	64K1
	Band structure and related properties: The band structure was determined theoretically by Kahn et al: Fig. 137.	65S18
	For discussions, see	66F3, 67F3
	Magnetoresistance, Shubnikov-deHaas effect. The conduction band consists of spheroids along [100] having 3 minima at X_3. The transverse and longitudinal effective electron mass: $m_t = 1.5\ m_0$ ($\pm 15\%$), $m_l = 6.0\ m_0$ ($\pm 30\%$).	67F3

Tab. 17. $SrTiO_3$. Elastic constants at RT

s_{11}	s_{12}	s_{13}	c_{11}	c_{12}	c_{13}	Method	Note	Reference
10^{-12} m² N⁻¹			10^{11} N m⁻²					
3.3	−0.74	8.4	3.48	1.01	1.19	composite-bar	c calculated from s	58p5
3.729	−0.909	8.091	3.181	1.025	1.236	pulse	s calculated from c	63B2
3.772 ±0.023	−0.926 ±0.010	8.233 ±0.040	3.156 ±0.027	1.027 ±0.027	1.215 ±0.006	pulse	s calculated from c	63W1

Tab. 18. $SrTiO_3$. n vs. λ at 21 °C. [57G1]

λ Å	n	λ Å	n	λ Å	n
4200	2.6050	5400	2.4386	6600	2.3771
4300	2.5810	5500	2.4312	6700	2.3737
4400	2.5585	5600	2.4245	6800	2.3703
4500	2.5394	5700	2.4182	6900	2.3674
4600	2.5236	5800	2.4122	7000	2.3645
4700	2.5101	5900	2.4069	7100	2.3617
4800	2.4970	6000	2.4019	7200	2.3590
4900	2.4846	6100	2.3971	7300	2.3564
5000	2.4734	6200	2.3928	7400	2.3538
5100	2.4636	6300	2.3886	7500	2.3514
5200	2.4548	6400	2.3846	7600	2.3490
5300	2.4464	6500	2.3807	7700	2.3468

Tab. 19. $SrTiO_3$. n vs. λ [65B9]

λ µm	n	λ µm	n
0.45	2.537	1.8	2.270
0.5	2.472	2.0	2.264
0.6	2.402	2.2	2.258
0.7	2.363	2.4	2.2524
0.8	2.340	2.6	2.2490
0.9	2.326	2.8	2.2395
1.0	2.315	3.0	2.2315
1.1	2.306	3.2	2.2236
1.2	2.299	3.4	2.2143
1.4	2.287	3.6	2.2058
1.6	2.279	3.8	2.1951

Figures p. 236ff.

Tab. 20. $SrTiO_3$. Π_{66} vs. λ at (27 ± 1) °C. [*57G1*]

λ Å	Π_{66} 10^{-13} m² N⁻¹	λ Å	Π_{66} 10^{-13} m² N⁻¹
4200	−3.69	6000	−4.92
4300	−3.74	6100	−4.99
4400	−3.78	6200	−5.05
4500	−3.99	6300	−5.12
4600	−3.965	6400	−5.13
4700	−4.13	6500	−5.18
4800	−4.09	6600	−5.22
4900	−4.22	6700	−5.29
5000	−4.33	6800	−5.52
5100	−4.32	6900	−5.48
5200	−4.41	7000	−5.555
5300	−4.51	7100	−5.62
5400	−4.59	7200	−5.77
5500	−4.575	7300	−5.73
5600	−4.62	7400	−5.78
5700	−4.69	7500	−5.79
5800	−4.79	7600	−5.825
5900	−4.85	7700	−5.98

Tab. 21. $SrTiO_3$. $\Pi_{21}-\Pi_{11}$ vs. λ at (27 ± 1) °C. [*57G1*]

λ Å	$\Pi_{21}-\Pi_{11}$ 10^{-13} m² N⁻¹	λ Å	$\Pi_{21}-\Pi_{11}$ 10^{-13} m² N⁻¹
4200	9.03	6000	9.95
4300	9.23	6100	9.94
4400	9.03	6200	9.91
4500	9.26	6300	9.84
4600	9.12	6400	9.82
4700	9.12	6500	9.88
4800	9.14	6600	9.96
4900	9.16	6700	9.92
5000	9.35	6800	9.98
5100	9.44	6900	9.99
5200	9.61	7000	9.91
5300	9.54	7100	9.92
5400	9.68	7200	9.94
5500	9.56	7300	9.99
5600	9.85	7400	10.05
5700	9.85	7500	9.90
5800	9.86	7600	9.92
5900	9.88	7700	10.02

Tab. 22. $SrTiO_3$ (single crystal). Effects of electrode material on the apparent conductivity [*65C6*]. Measurements were made by the two terminal method at T = 130 °C, t = 24 hours after the application of the field E = 100 kV m⁻¹

Electrode material	σ [Ω^{-1} m⁻¹] after 24 h at 130 °C	Form of σ vs. t curve
Au	$4{\cdot}8 \cdot 10^{-7}$	Fall then rise
Ag	$8{\cdot}8 \cdot 10^{-8}$	As for gold
Sn	$8{\cdot}8 \cdot 10^{-9}$	Fall followed by slow rise but without saturation
Cr	$6{\cdot}0 \cdot 10^{-11}$	Continuous fall tending toward steady value
Cd	$9{\cdot}5 \cdot 10^{-11}$	Similar to chromium
Al	$2{\cdot}9 \cdot 10^{-10}$	Similar to chromium (for a field of 400 kV m⁻¹ behavior is like that of gold)

Tab. 23. $SrTiO_3$ (single crystal). The 300 °K and 2 °K Hall coefficient R_H and Hall mobility μ_H values and the 300 °K electron concentrations for semiconductive single crystals. [*67T6*]. In the first column, (Nb) means Nb-doped samples, the other samples are reduced ones

Sample	300 °K R_H 10^{-6} m³ C⁻¹	300 °K μ_H 10^{-4} m² V⁻¹ sec⁻¹	2 °K R_H 10^{-6} m³ C⁻¹	2 °K μ_H 10^{-1} m² V⁻¹ sec⁻¹	$n = \dfrac{1}{eR_H\,(300\,°K)}$ m⁻³
5	0.26	6.5	0.25	1.0	$2.4 \cdot 10^{25}$
2	0.62	5.2	0.77	1.8	$1.0 \cdot 10^{25}$
3	1.8	7.2	3.9	2.7	$3.5 \cdot 10^{24}$
6	5.3	8.0	11.0	3.1	$1.2 \cdot 10^{24}$
12	14.0	8.0			$4.5 \cdot 10^{23}$
9	23.0	5.8			$2.7 \cdot 10^{23}$
13(Nb)	0.22	5.5	0.22	3.3	$2.8 \cdot 10^{25}$
8(Nb)	0.58	4.8	0.63	8.2	$1.1 \cdot 10^{25}$
10(Nb)	3.4	6.2	3.3	12.0	$1.8 \cdot 10^{24}$
14(Nb)	14.0	6.7	11.0	13.0	$4.5 \cdot 10^{23}$
15(Nb)	22.0	5.4	18.0	19.0	$2.8 \cdot 10^{23}$
11(Nb)	44.0	6.0	33.0	22.0	$1.4 \cdot 10^{23}$

Tab. 24 see page 50

Tab. 25. $SrTiO_3$. Susceptibility in pure and reduced single crystals [66F2]. $\Delta\chi_{magn\,g}$ represents the contribution from the charge carriers; $\Delta\chi_{magn\,g}$ is obtained by measuring the $\chi_{magn\,g}$ of reduced crystals and subtracting the "pure" diamagnetic and Van Vleck contributions. N = carrier concentration; T_{deg} = degeneracy temperature; m^* = density-of-state effective mass

Sample	N at 4.2 °K m^{-3}	T_{deg} °K	$\chi_{magn\,g}$ or $\Delta\chi_{magn\,g} \cdot 10^{-7}$ cm³ g⁻¹	300 °K	78 °K	4.2 °K	m^* at 4.2 °K [m_0]
pure	—	—	χ	−1.02	−1.00	−0.92	—
28 h, 950 °C hydrogen	$6 \cdot 10^{24}$	28	$\Delta\chi_1$	+0.037	+0.073	—	—
5 h, 1200 °C hydrogen (carbon boat)	$7.5 \cdot 10^{25}$	148	$\Delta\chi_2$	+0.270	+0.523	+0.928	5.1
reoxidized 18 h, 700 °C, air	—	—	χ	−1.016	−1.012	−0.919	—
27 h, 1370 °C hydrogen (carbon boat)	$5.3 \cdot 10^{26}$	550	$\Delta\chi_3$	+1.704	+1.763	+1.719	4.9

Tab. 27. $SrTiO_3$. The frequency of the lowest transverse optic mode at $q = 0$ for five different temperatures. [62C4]

T °K	ν 10^{12} sec⁻¹ Neutron	Far infrared
90	1.23 ± 0.03	1.2[a]
142	1.72 ± 0.04	
203	2.24 ± 0.05	
296	2.73 ± 0.05	3.0[a] 2.63[b]
430	3.32 ± 0.07	

[a] [62B2] [b] [62S12]

Tab. 26. $SrTiO_3$. Summary of the properties of ESR spectrum in $SrTiO_3$ for various doped paramagnetic ions

Para-magnetic center	Site	S	$\mathscr{H}$	ν GHz	T °K	g-factor $g_\parallel$	$g_\perp$	FS D, E, a [10^{-2} m⁻¹]	HFS I	^nA [10^{-2} m⁻¹]	Ref.	Literature
Cr^{3+}	Ti^{4+}	3/2	(5)	9	80	1.9788 ± 0.007	(isotropic)	$D = 2 \pm 0.3$, $E = 0$	3/2	$^{53}A = 0$	f)	58M7
					300	1.9780 ± 0.007	(isotropic)	$D = 0$, $E = 0$		$^{53}A = 16.2 \pm 0.3$		62M6
Mn^{4+}	Ti^{4+}	3/2	(5)	10	77	1.994 ± 0.001	(isotropic)	$D = +1.0$, $E = 0$	5/2	$^{55}A = -69.4 \pm 1$		59M4
					RT	1.994 ± 0.001	(isotropic)	$D = -0.7$, $E = 0$		$^{55}A = -69.4 \pm 1$		
Fe^{3+}	Ti^{4+}	5/2	(7)	9	1.9	2.004 ± 0.001	(isotropic)	$D = +17.9 \pm 1.0$, $E = 0$ $a = -230 \pm 10$, $E = 0$			a)	59D2
					4.2	2.004 ± 0.001	(isotropic)	$D = +16.1 \pm 0.7$, $E = 0$ $a = -225.6 \pm 1.9$			b)	
					77	2.004 ± 0.001	(isotropic)	$D = +7.3 \pm 0.3$, $E = 0$ $a = -220.8 \pm 1.1$			f)	58M8
					300	2.004 ± 0.001	(isotropic)	$D = 1.0$, $E = 0$ $a = -197.7 \pm 0.7$			g)	
Ni^{2+}	Ti^{4+}	1	(4)	10	80	2.204 ± 0.001	(isotropic)				c)	62R3
Ni^{1+} or Ni^{3+}	Ti^{4+}	1/2	(2)	10	20							
					80	2.029 ± 0.001	2.352 ± 0.001				d)	62R3
					203						e)	

Ni²⁺	Ti⁴⁺	1	(4)	10	80						
Ni^{1+} or Ni^{3+}	Ti^{4+}	1/2	(2)	10	20	2.029 ± 0.001	2.352 ± 0.001			e)	
					80						
					203						

Para-magnetic center	Site	S	$\mathscr{H}$	ν GHz	T °K	g-factor $g_{\parallel}$	$g_{\perp}$	FS D, E, a [10^{-2} m^{-1}]		HFS I	$^{n}A_{\parallel}$, $^{n}A_{\perp}$ [10^{-2} m^{-1}]	Ref.	Literature
Ni^{3+}	Ti^{4+}	1/2	(2)	10	4.2	2.110 ± 0.002	2.213 ± 0.002					e)	*62R3*
					20	2.136 ± 0.001	2.202 ± 0.001						
					80	2.172 ± 0.001	2.184 ± 0.001						
					203	(isotropic)	2.180 ± 0.002						
Ce^{3+}	—	1/2	(2)	10	4.2	3.005 ± 0.005	1.118 ± 0.003					e)	*62R3*
Nd^{3+}	—	1/2	(2)	10	4.2	2.609 ± 0.003	2.472 ± 0.003					e)	*62R3*
				16	2	2.61 ± 0.01	2.470 ± 0.005						*62R2*
				35		2.62 ± 0.01	2.470 ± 0.005						
Yb^{3+}	—	1/2	(3)	16	2	2.11 ± 0.01	2.780 ± 0.005						*62R2*
				35		2.10 ± 0.005				1/2 5/2	$\lvert ^{171}A_{\parallel} \rvert = 530 \pm 20$ $\lvert ^{171}A_{\perp} \rvert = 720 \pm 5$ $\lvert ^{173}A_{\perp} \rvert = 211 \pm 5$		
				16	50	2.18 ± 0.01	2.720 ± 0.005						
				35		2.17 ± 0.005	2.720 ± 0.005						
				35	65	(2.25)	2.70 ± 0.01						
						g (isotropic)	FS [10^{-2} m^{-1}] b_{20}	b_{40}	b_{60}				
Eu^{2+}	—	7/2	(8)	16	2	1.99 ± 0.001	−10 ± 4	106.6 ± 2	6.7 ± 2	5/2 5/2	$\lvert ^{151}A_{\parallel} \rvert = 36.2$ $\lvert ^{153}A_{\perp} \rvert = 17.6$	f)	*62R2*
					300	1.99 ± 0.001	0	105.9 ± 2	1.1 ± 2				
Gd^{3+}	Sr^{2+}	7/2	(8)	16	2	1.992 ± 0.002	−362.5 ± 0.5	−3.2 ± 0.5	1.4 ± 0.5			f)	*62R2*
				12, 18	4.2	1.992 ± 0.002	−362.5 ± 0.5	−3.24 ± 0.5	1.4 ± 0.5			h)	*62R1*
					77	1.992 ± 0.002	−233.6 ± 0.5	−4.8 ± 0.5	−0.25 ± 0.5				
					300	1.992 ± 0.002		−5.7 ± 0.2	0.5 ± 0.3				

a) $\xi = [100]$, $\eta = [010]$, $\zeta = [001]$.
b) Deviations from spin Hamiltonian (7) is ascribed to a covalent bonding by Müller. However, Aisenberg et al. find a negligible contribution of the covalent bonding. [*59A1*].
c) Spectrum is due to a double quantum absorption between $S_z = -1$ and $S_z = +1$ levels.
d) At least fifteen inequivalent sites are observed.
e) Three inequivalent spectra are observed with axes parallel to the cubic [100], [010] and [001].
f) Effects of temperature and pressure on Cr^{3+}, Fe^{3+}, Eu^{2+}, and Gd^{3+} spectra. [*64R2*].
g) Fe^{3+} spectra due to nearest charge compensation. [*64K7*].
h) Electric field dependence of Gd^{3+} spectra. [*66S3*].

Tab. 24. $SrTiO_3$ (ceramics containing Ba or Ca in mol%). Superconductive properties of $(Ba_xSr_{1-x})TiO_3$ and $(Ca_xSr_{1-x})TiO_3$ [67S8]. H_{c1} is the point at which the magnetization curve first deviates from linearity; $H_{c1}(0)$ is the extrapolated value for $T \to 0$ °K.
N = Carrier concentration Θ_c = superconducting transition temperature

% Ba or Ca	N 10^{25} m^{-3}	Θ_c °K	$H_{c1}(0)$ Oe	% Ba or Ca	N 10^{25} m^{-3}	Θ_c °K	$H_{c1}(0)$ Oe
—	2.7	0.18		10.0	4.2	0.25	
—	5.8	0.30	2.8	12.5	4.5	<0.10	
—	6.4	0.25	2.8	2.5 (Ca)	5.0	0.32	
—	1.7	0.10		5.0	9.2	0.30	
—	12.0	0.17		7.5	74.0	<0.06	
—	23.0	0.10		7.5	8.7	0.43	(3.5)[a]
2.5 (Ba)	6.0	0.52		7.5	0.2	<0.06	
2.5	0.3	0.23		7.5	0.6	0.37	
5.0	6.7	0.50	3.9	7.5	33.0	<0.07	
7.5	7.0	0.29		7.5	2.0	0.48	
7.5	0.05	0.22		7.5	0.06[b]	<0.06	
7.5	34.0	0.09		10.0	9.3	0.39	
7.5	0.5	0.25		20.0	13.0	0.29	
7.5	2.3	0.27		30.0	6.7	0.50	1.9
7.5	15.0	0.45		30.0	0.6	<0.05	

Nr. 1A-7 $CdTiO_3$, Cadmium titanate

1a	$CdTiO_3$ was reported by SMOLENSKII in 1950 to be ferroelectric below 50 ··· 60 °K. In 1950 HULM et al. denied its ferroelectricity but HEGENBARTH supported SMOLENSKII's findings.	*50S7, 50H2, 59H4*
b	(see phase table below)	[a] *50S7*; [b] *57K1*
	Lattice constants: $a = 5.348$ Å, $b = 7.615$ Å, $c = 5.417$ Å at RT. The relation between the orthorhombic unit cell and the pseudo-cubic monoclinic cell is the same as in the case of $NaTaO_3$; see Fig. 21.	*50S7* *57K1*
2	Flux method (flux: 40 wt% NaCl + 40 wt% $NaBO_2$ + 20 wt% Na_2CO_3).	
3	$Z = 4$. Crystal structure in phase I: Tab. 28; Fig. 138.	*57K1*
5a	Dielectric constant: $\varkappa = 250$ at RT. $\varkappa = C/(T - \Theta_p)$, $C = 4.5 \cdot 10^4$ °K.	
b	Effect of E_{bias} on $\varkappa$: Fig. 139.	*50S7, 50H2*

phase	II	I
state	(F)[a]	
crystal system		orthorhombic[b]
space group		$Pc2_1n$[b]$-C_{2v}^9$
Θ	−223··· −213 °C	

Tab. 28. $CdTiO_3$. Fractional coordinates of atoms in the unit cell. [57K1]

		Positions				Estimated error
Cd	x:	$0 + 0.006$	$0 - 0.006$	$\frac{1}{2} + 0.006$	$\frac{1}{2} - 0.006$	± 0.002
	y:	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	
	z:	$0 + 0.016$	$0 - 0.016$	$\frac{1}{2} - 0.016$	$\frac{1}{2} + 0.016$	± 0.002
Ti	x:	$\frac{1}{2} + 0.005$	$\frac{1}{2} - 0.005$	$0 + 0.005$	$0 - 0.005$	± 0.005
	y:	0	$\frac{1}{2}$	$\frac{1}{2}$	0	
	z:	$0 - 0.065$	$0 + 0.065$	$\frac{1}{2} + 0.065$	$\frac{1}{2} - 0.065$	± 0.010
O(1)	x:	$0 - 0.03$	$0 + 0.03$	$\frac{1}{2} + 0.03$	$\frac{1}{2} - 0.03$	± 0.015
	y:	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	$\frac{1}{4}$	± 0.025
	z:	$\frac{1}{2} + 0.05$	$\frac{1}{2} - 0.05$	$0 + 0.05$	$0 - 0.05$	± 0.015
O(2)	x:	$\frac{1}{4} + 0.05$	$\frac{1}{4} - 0.05$	$\frac{3}{4} - 0.05$	$\frac{3}{4} + 0.05$	± 0.005
	y:	$0 - 0.03$	$0 - 0.03$	$\frac{1}{2} - 0.03$	$\frac{1}{2} - 0.03$	± 0.015
	z:	$\frac{1}{4} + 0.06$	$\frac{3}{4} + 0.06$	$\frac{3}{4} - 0.06$	$\frac{1}{4} - 0.06$	± 0.015
O(3)	x:	$\frac{1}{4} + 0.05$	$\frac{1}{4} - 0.05$	$\frac{3}{4} - 0.05$	$\frac{3}{4} + 0.05$	± 0.005
	y:	$\frac{1}{2} + 0.07$	$\frac{1}{2} + 0.07$	$0 + 0.07$	$0 + 0.07$	± 0.015
	z:	$\frac{1}{4} + 0.06$	$\frac{3}{4} + 0.06$	$\frac{3}{4} - 0.06$	$\frac{1}{4} - 0.06$	± 0.015

[a]) This specimen is not spherical, so that the value of $H_{c1}(0)$ quoted is only approximate.
[b]) Hall coefficient appeared to be affected by magnetic history of specimen at liquid helium temperature.

Nr. 1A-8 $BaTiO_3$, Barium titanate

(Responsible authors for this section are as follows: Ikeda, Nakamura, Nomura, Sawaguchi, Shiozaki and Toyoda, abbreviated as INaNoSaShiTo).

1a The anomalous dielectric properties of $BaTiO_3$ were discovered on ceramic specimens independently by Wainer and Solomon in 1942, by Ogawa in 1944 and by Wul in 1945. The ferroelectric activity of $BaTiO_3$ was reported independently by von Hippel and co-workers in 1944 and by Wul in 1946. The structural change associated with the cubic-tetragonal phase transition was observed, by means of x-rays, by Megaw in 1945, independently of the above dielectric studies. *42W1, 44O1, 45W1, 44V2, 46W2, 45M1*

b

phase	IV[a]	III[a]	II[b]	I[b]	
state	F[a]	F[a]	F[c]	P[b]	
crystal system	rhombohedral[a]	orthorhombic[a]	tetragonal[b]	cubic[b]	hexagonal[d]*
space group	R3m-C_{3v}^5 [a]	Amm2-C_{2v}^{14} [a]	P4mm-C_{4v}^1 [b]	Pm3m-O_h^1 [b]	C63/mmc-D_{6h}^4 [d]

Θ: −90[a] 5[a] 120[b]** 1460[d] °C

[a] 49K2, 49R1; [b] 45M1; [c] 46V1, 46W1; [d] 55R1

P_s || [001] in phase II (along [100] of phase I).
P_s || [001] in phase III (along [110] of phase I).
P_s || [111] in phase IV (along [111] of phase I).
The directions of P_s are illustrated along with lattice distortions in Fig. 140.
$T_{melt} = 1618$ °C. *51W2*
Tetragonal form (phase II): $\varrho = 6.02 \cdot 10^3$ kg m^{-3} (calculated from lattice constants)
$a = 3.9920$ Å, $c = 4.0361$ Å at 20 °C. *51R1*
Transparent, light brown.
Hexagonal form: $a_{hex} = 5.735$ Å, $c_{hex} = 14.05$ Å at RT. *48B3*
$\varrho = (6.1 \pm 0.1) \cdot 10^3$ kg m^{-3}.

2a Crystal growth: Flux method (flux KF[a]) or TiO_2-rich melt[b]). *[a] 54R1, [b] 65S8*
Pulling method (top-seeded solution growth technique using excess TiO_2 as the solvent). *63L3*
Melting method (with limited success). *50V2*
Tab. 29; Fig. 141.

b Crystal forms: For butterfly-type: Fig. 142.
For chunky type: Fig. 143.
For hexagonal form: Fig. 144.

3 Crystal structure of phase I: $Z = 1$. Tab. 30.
Crystal structure of phase II: $Z = 1$. Tab. 31.
Crystal structure of phase III: $Z = 2$. Tab. 32; Fig. 145, 146; Tab. 33.
Crystal structure of phase IV: $Z = 1$.
Crystal structure of hexagonal form: $Z = 6$. Tab. 34, 35; Fig. 147.

4 Lattice constants of phase I, II, III, and IV:
Phase I: $a = 3.996$ Å at 120 °C. *47M3*
Phase II: $a = 3.9920$ Å, $c = 4.0361$ Å at 20 °C. *51R1*
Phase III: $a = 3.990$ Å, $b = 5.669$ Å, $c = 5.682$ Å at −10 °C. *57S2*
Phase IV: $a = 4.001$ Å, $\alpha = 89° 51'$ at −168 °C. *57J2*
Thermal expansion: Fig. 148, 149; Tab. 36, 37; Fig. 150.
Lattice distortion due to p: Fig. 151.

5a Dielectric constant: Fig. 152, 153, 154, 192.
Dielectric dispersion: Fig. 155 ··· 159.
Further data from optical measurements: Fig. 201; Tab. 42.
Effect of p on $\varkappa$: Fig. 160, 161, 162.
Phase diagram in regard to p: Fig. 163, 164.
Effect of E_{bias} on Θ_f: $d\Theta_f/dE_{bias} = 1.43 \cdot 10^{-5}$ °K V^{-1} m; *53M2*
on $\varkappa$: Fig. 165.

b Non-linear dielectric properties: Fig. 166.
$\xi = -5.5 \cdot 10^8$ J C^{-4} m^5, $\zeta = 1.7 \cdot 10^{10}$ J C^{-6} m^9. *53M2*

* The transition from the hexagonal form to the cubic one is very sluggish and the hexagonal form can be produced by rapid cooling from above 1460 °C.
** In most papers this Curie point has been reported to be about 120 °C, but it seems to be about 130 °C for pure $BaTiO_3$ [*65J2*].

	Nr. 1A-8 $BaTiO_3$ continued	
5c	Spontaneous polarization: Fig. 167, 168, 169. Coercive field: Fig. 170, 171, 172. Effect of p on P_s: Fig. 173.	
d	Electrocaloric effect: Fig. 174. Pyroelectricity: Fig. 175.	
6a	Specific heat: Fig. 176, 177. Transition heat, transition entropy: Tab. 38.	
b	Thermal conductivity: Fig. 178, 179.	
7a	Piezoelectricity: Tab. 39, 40; Fig. 180 ··· 183.	
b	Electrostriction: Fig. 184, 185.	
8a	Elastic compliances and stiffnesses: Tab. 41. See also Tab. 40. Fig. 186 ··· 193.	
b	Non-linear elastic properties: Fig. 194.	
9a	Refractive indices: Fig. 195, 196, 197. Birefringence: Fig. 198, 199. Reflection and absorption: (i) Far-infrared region. Fig. 200, 201; Tab. 42. (ii) Infrared region. Fig. 202, 203, 204. (iii) Visible region. Fig. 205, 206, 207. (iv) Ultraviolet region. Fig. 208; Tab. 43; Fig. 209, 210, 211. For the effect of E_{bias} on the absorption edge, see	*67G1*
b	Linear electrooptic effect: Fig. 212 ··· 215. Quadratic electrooptic effect: $(M_{11} - M_{12}) = (+ 0.13 \pm 0.02)\ m^4\,C^{-2}$ at 408 ··· 433 °K, measured at 6328 Å.	*64G3*
d	Faraday rotation: Fig. 216; Tab. 44.	
e	Non-linear optical properties: Susceptibility for SHG (second harmonic generation) (relative values, see Sec. I C): $d_{15} = 35 \pm 3$, $d_{31} = 37 \pm 3$, $d_{33} = 14 \pm 1$, determined with the Nd-doped $CaWO_4$ laser beam. Fig. 217.	*64M2*
f	Raman scattering: Fig. 218.	
g	Luminescence: Fig. 219, 220.	
10	Conductivity of as-grown crystals and ceramics: The data vary from sample to sample depending on the purity and the method of preparation: only representative data are given here. Fig. 221 ··· 225. Conductivity associated with doping or reduction (including PTC (Positive Temperature Coefficient) or resistivity: $d\varrho/dT > 0$): Fig. 226 ··· 230. Reference papers on PTC anomaly: Tab. 45. Piezoresistivity: Fig. 231, 232. For additional data, see	*59S1, 63M1, 67G4*
	Breakdown strength: Fig. 233, 234. For additional data, see	*58I3, 59F1, 64K3, 64U1*
	Photoconductivity and photoemission: Fig. 235, 236. Other transport properties: In n-type single-domain crystals, the electron mobility is anisotropic at RT; $\mu_{\perp c} \approx 1.2 \cdot 10^{-4}\ m^2\,V^{-1}\,sec^{-1}$, and $\mu_c \approx 0.13 \cdot 10^{-4}\ m^2\,V^{-1}\,sec^{-1}$ at 26 °C.	*67B2*
	In n-type single-domain crystals, the energy separation ($\Delta u = 10^{-2} \cdots 10^{-1}$ eV) between the c-axis conduction band minima and the a-axis conduction band minima has been estimated vs. T.	*67B2*
	In n-type single-domain crystals, the density-of-state mass $m^* = (6.5 \pm 2)\,m_0$. Data are available on the Hall coefficient and conductivity of single domain crystals having donor concentrations of $N = 8.5 \cdot 10^{24}\ m^{-3}$ and of $N = 2.5 \cdot 10^{23}\ m^{-3}$. Fig. 237. Seebeck-effect: Fig. 238.	*67B2* *67B2*
12b	ESR: Tab. 46; Fig. 239 ··· 243.	
c	Mössbauer effect: Fig. 244 ··· 247.	
13b	Diffuse X-ray scattering: Fig. 248, 249, 250. Inelastic neutron scattering: Fig. 251.	

14a	Domain structure: Domains have been observed by various methods: polarized light[a]), X-rays[b]), electron microscope[c]), etching method[d]), powder pattern method[e]), and decoration method[f]). Fig. 252 ··· 255.	a) *48M1, 49F1, 52M3* b) *63B13, 64N1, 65C3, 64L1* c) *62T1, 63B9, 67R4, 64T2, 66R5, 67R2* d) *55H2* e) *59P1* f) *66S8*
b	Domain wall motion: Domain wall motion has been observed optically[a]) and by repeated differential etching.[b]) The domain shapes in motion depend on the applied field and temperature.[c]) Fig. 256.	a) *59M2, 60S2* b) *63S13* c) *63S13*
	The wall velocity is proportional to exp $(-\delta/E)$ at relatively low field. δ = activation field for domain wall motion. Fig. 257 ··· 267.	*58M4, 59M3*
15	Surface layer: The first suggestion about the existence of surface layers of $BaTiO_3$ crystals was made by KÄNZIG[a]) on the basis of electron diffraction studies of very small particles of $BaTiO_3$[b]). The dependence of the following quantities on the thickness of the crystals has been observed as evidence of the existence of surface layers: domain wall velocity[c]), dielectric constant[d]), optical absorption coefficient[e]) and electroluminescence spectra[f]). Pyroelectric current was observed above the Curie point and discussed in connection with surface layers[g]). A few models of surface layers have been proposed[h]). According to TANAKA and HONJŌ[i]), the surface layer, if it exists, seems to be very thin.	a) *55K1* b) *54A1* c) *56M4, 61M2, 65C1* d) *61S4, 62C3* e) *60C3* f) *58H1, 65B7, 66B6* g) *56C1* h) *56M4, 61F2, 59D3, 65C1* i) *64T2*
16	Radiation damage: Fig. 268, 269.	
17	Energy band structure: Fig. 270.	

Tab. 29. $BaTiO_3$. Solubility in KF solution. [*54K1*]

T	1000	1050	1100	1150	1200	1250	1300	°C
$BaTiO_3$	4	6	9	12.5	17	22.5	28.5	mole %

Tab. 30. $BaTiO_3$. Fractional coordinates of atoms in the unit cell of phase I. [*52M2*]

	x	y	z
Ba	0	0	0
Ti	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
O	$\frac{1}{2}$	$\frac{1}{2}$	0
	$\frac{1}{2}$	0	$\frac{1}{2}$
	0	$\frac{1}{2}$	$\frac{1}{2}$

Tab. 31. $BaTiO_3$. Shift of atoms in fractional coordinates of phase II from the positions of phase I. [*51K1*], [*55F1*], [*61E3*]

δz_{Ti}	$\delta z_{O(1)}$	$\delta z_{O(2)}$	Ba		Ti		O(1)		O(2)			References
			B_{11}	B_{33}	B_{11}	B_{33}	B_{11}	B_{22}	B_{11}	B_{22}	B_{33}	
0.014	−0.032	0	0.48		0.13		0.13		0.48			*51K1*
0.014	−0.023	−0.014	0.273		0.152		0.334		0.267			*55F1*
0.015	−0.024	−0.020	0.27	0.28	0.53	0.21	0.90	0.08	0.60	0.49	0.07	*61E3*
0.012	−0.026	0	0.27	0.28	0.46	0.30	0.90	0.50	0.60	0.90	0.90	*61E3*

The positions of atoms in the unit cell are Ba at (0, 0, 0), Ti at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} + \delta z_{Ti})$, O(1) at $(\frac{1}{2}, \frac{1}{2}, \delta z_{O(1)})$ and O(2) at $(\frac{1}{2}, 0, \frac{1}{2} + \delta z_{O(2)})$.

Tab. 32. $BaTiO_3$. Fractional coordinates of atoms in the unit cell of phase III. [57S2]

	x	y	z
Ba	0	0	0
	0	$\frac{1}{2}$	$\frac{1}{2}$
Ti	$\frac{1}{2}$	0	$\frac{1}{2} + \delta z_{Ti}$
	$\frac{1}{2}$	$\frac{1}{2}$	δz_{Ti}
O(1)	0	0	$\frac{1}{2} + \delta z_{O(1)}$
	0	$\frac{1}{2}$	$\delta z_{O(1)}$
O(2)	$\frac{1}{2}$	$\frac{1}{4} + \delta y_{O(2)}$	$\frac{1}{4} + \delta z_{O(2)}$
	$\frac{1}{2}$	$\frac{3}{4} + \delta y_{O(2)}$	$\frac{3}{4} + \delta z_{O(2)}$
	$\frac{1}{2}$	$\frac{3}{4} - \delta y_{O(2)}$	$\frac{1}{4} + \delta z_{O(2)}$
	$\frac{1}{2}$	$\frac{1}{4} - \delta y_{O(2)}$	$\frac{3}{4} + \delta z_{O(2)}$

$\delta z_{Ti} = +0.010$; $\delta z_{O(1)} = -0.010$; $\delta z_{O(2)} = -0.013$; $\delta y_{O(2)} = +0.003$.

Tab. 33. $BaTiO_3$. Comparison of atomic shifts in phase III and phase II with respect to different origins. The coordinate of atoms of [55F1] and [57S2] are used for phase II and III, respectively. [57S2]

		Orthorhombic	Tetragonal
		Ba at (000)	
δz	Ti	+0.06 Å	+0.06 Å
	O(1)	−0.06 Å	−0.09 Å
	O(2)	−0.07 Å	−0.06 Å
$\delta y_{O(2)}$		±0.02 Å	—
		Origin is chosen to give $\delta z_{O(2)} = 0$	
δz	Ti	+0.13 Å	+0.15 Å
	Ba	+0.07 Å	+0.09 Å
	O(1)	+0.02 Å	−0.03 Å

Tab. 34. $BaTiO_3$. Fractional coordinates of atoms in the unit cell of hexagonal structure. [48B3]

2Ba(1) at (b),
4Ba(2) at (f), $z = 0.097$,
2Ti(1) at (a),
4Ti(2) at (f), $z = 0.845$,
6O(1) at (h), $x = 0.522$,
12O(2) at (k), $x = 0.836$, $z = 0.076$

Tab. 35. $BaTiO_3$. Interatomic distances of hexagonal structure. [48B3]

in the Ti_2O_9 group

O(1) − O(1) = 2.49 Å	in the shared face.
= 3.25 Å	in the same layer but the atoms do not belong to the same shared face.
O(2) − O(2) = 2.91 Å	
O(1) − O(2) = 2.91 Å	
Ti(2) − O(1) = 1.96 Å	
Ti(2) − O(2) = 2.02 Å	

in the TiO_6 octahedra

O(2) − O(2) = 2.82 Å	in the same layer.
O(2) − O(2) = 2.69 Å	between adjacent layers.
Ti(1) − O(2) = 1.95 Å	

Tab. 36. $BaTiO_3$. Lattice constants and unit cell volume at various T. [51R1]

T °C	a Å	b Å	c Å	V Å³
+ 20	3.9920	3.9920	4.0361	64.317
+ 4	3.9910	3.9911	4.0357	64.282
Θ_{III-II}				
+ 4	4.0185	3.9860	4.0162	64.319
− 99	4.0170	3.9750	4.0150	64.093
Θ_{IV-III}				
− 99	4.0015	4.0015	4.0020	64.079
−160	3.9996	3.9996	3.9997	63.981

Accuracy of measurement below RT was ±0.0007 Å.

Tab. 37. $BaTiO_3$. Linear thermal expansion coefficients along a, b, and c axes. [51R1]

T °C	α_a 10^{-6} °C^{-1}	α_b 10^{-6} °C^{-1}	α_c 10^{-6} °C^{-1}
+20 ··· + 4	15.7	15.7	6.2
+ 4 ··· − 99	4.9	28.4	−0.9
−99 ··· −160	7.8	7.8	8.2

Tab. 38. $BaTiO_3$. Transition heats and transition entropies

Transition	ΔQ_m cal mol^{-1}	ΔS_m cal mol^{-1} °K^{-1}	References
IV → III	8 ± 2	0.04	52S5
	14.3	0.07	52V1
	12	0.06	52T1
III → II	22 ± 4	0.076	52S5
	15.5	0.054	52V1
	16	0.058	52T1
II → I	50 ± 5	0.125	52S5
	47	0.12	52V1
	47	0.12	48B1

Tab. 39. $BaTiO_3$ (single crystal and ceramic). Piezoelectric constants and electromechanical coupling factor. [66b1]

	d_{15}	d_{31}	d_{33}	g_{15}	g_{31}	g_{33}	k_{15}	k_{31}	k_{33}	k_p	e_{15}	e_{31}	e_{33}	h_{15}	h_{31}	h_{33}	T	References
	10^{-12} CN^{-1}			10^{-3} m^2 C^{-1}							C m^{-2}			10^8 N C^{-1}			°C	
single crystal	392	−57.7 −34.5 −33.3 −103.3	132 85.6 316.6	15.3	−23.1	57.6	0.570	0.315	0.560								20 25 RT	*50C2* *58B2* *59H7* *51B1*
ceramic	270 260	−79 −78	191 190	18.8 20.2	−4.7 −5.2	11.4 12.6	0.476 0.48	0.208 0.212	0.493 0.50	0.378 0.36	11.6 11.4	−4.4 −4.35	18.6 17.5	10.3 11.5	−3.5 −3.9	14.8 15.6	25 25	*56B3* *64b1*

Tab. 40. $BaTiO_3$ (ceramic, plain and modified, commercial). Dielectric, piezoelectric, electromechanical and elastic constants (at 25 °C, except for $Ca_{0.12}Pb_{0.08}Ba_{0.80}TiO_3$). [66b1]

Composition	$\varkappa_{33}^T$	d_{15}	d_{31}	d_{33}	g_{15}	g_{31}	g_{33}	k_{15}	k_{31}	k_{33}	k_p	s_{11}^E	s_{12}^E	s_{66}
		10^{-12} CN^{-1}			10^{-3} m^2 C^{-1}							10^{-12} m^2 N^{-1}		
$BaTiO_3$	1350 ⋯ 1700		−56	130 ⋯ 160								8.47	−2.38	21.7
$Ca_{0.03}Ba_{0.97}TiO_3$	1380		−53	135								8.20	−2.45	21.3
$Ca_{0.05}Ba_{0.95}TiO_3$ (ceramic B)[a]	1200	242	−58	149	21.0	−5.5	14.1	0.48	0.194	0.48	0.33	8.6	−2.6	22.4
$Ca_{0.09}Ba_{0.91}TiO_3$	910		−41	118								8.00	−2.40	20.79
$Pb_{0.04}Ba_{0.96}TiO_3$	1000		−38	105								8.77	−2.58	22.7
$Pb_{0.05}Ba_{0.95}TiO_3$	1180		−53	129								9.09	−2.64	23.64
$Ca_{0.06}Pb_{0.04}Ba_{0.90}TiO_3$	800		−40	115								8.06	−2.34	20.8
$Ca_{0.08}Pb_{0.08}Ba_{0.84}TiO_3$	600		−29	80								7.63	−2.87	20.0
$Ca_{0.08}Pb_{0.12}Ba_{0.80}TiO_3$	450		−20	60		−5.0	15.0	0.30	0.113	0.34	0.19	7.8	−2.3	20.2
$Ca_{0.12}Pb_{0.08}Ba_{0.80}TiO_3$	600		−35	90		−7.3	18		0.12	0.30	0.22	13		

	$\varkappa_{11}^T$	$\varkappa_{11}^S$	$\varkappa_{33}^S$	e_{15}	e_{31}	e_{33}	s_{11}^D	s_{33}^E	s_{33}^D	s_{12}^D	s_{13}^E	s_{13}^D	s_{44}^E	s_{44}^D
				C m^{-2}			10^{-12} m^2 N^{-1}							
$Ca_{0.05}Ba_{0.95}TiO_3$ (ceramics B)[a]	1300	1000	910	10.9	−3.1	13.5	8.3	9.1	7.0	−2.9	−2.7	−1.9	22.2	17.1
$Ca_{0.08}Pb_{0.12}Ba_{0.80}TiO_3$			395				7.7	8.1	7.15	−2.4				

	h_{15}	h_{31}	h_{33}	c_{11}^E	c_{11}^D	c_{33}^E	c_{33}^D	c_{12}^E	c_{12}^D	c_{13}^E	c_{13}^D	c_{44}^E	c_{44}^D	c_{66}
	10^8 N C^{-1}			10^9 N m^{-2}										
$Ca_{0.05}Ba_{0.95}TiO_3$ (ceramics B)[a]	12.3	−3.8	16.7	158	159	150	177	69	70	67.5	62	45	58.5	45

[a]) Trade Mark: Clevite Corporation, Cleveland, Ohio, USA.

Tab. 41. $BaTiO_3$ (single crystal and ceramics). Elastic constants. [66b1]

	s_{11}^E	s_{11}^D	s_{33}^E	s_{33}^D	s_{12}^E	s_{12}	s_{13}^E	s_{13}^D	s_{44}^E	s_{44}^D	s_{66}	T °C	References
	10^{-12} m^2 N^{-1}												
single crystal	9.26 11.2 8.05	7.25	15.7	10.8	−2.35	−3.15	−5.24	−3.26	18.4	12.4	8.84	25 RT 25	*50C2* *51B1* *58B2*
ceramics	8.55 9.1	8.18 8.7	8.93 9.5	6.76 7.1	−2.61 −2.7	−2.98 −3.0	−2.85 −2.9	−1.95 −1.9	23.3 22.8	18.3 17.5	22.3 23.6	25 25	*56B3* *64b1*
	c_{11}^E	c_{11}^D	c_{33}^E	c_{33}^D	c_{12}^E	c_{12}^D	c_{13}^E	c_{13}^D	c_{44}^E	c_{44}^D	c_{66}		
	10^{9} N m^{-2}												
single crystal	275.1	282.6 206	164.9	178.1	179.0	186.5 140	151.6	141.6	54.34	80.64 126	113.1	25 RT	*66b1, 58B2* *51B1*
ceramics	166 150 165.6	168 150	162 146	189 171 180.7	76.6 66	78.2 68	77.5 66	71.0 57	42.9 44 42.48	54.6 57 53.02	44.8 43 45.65	25 25 25	*56B3* *64b1* *55H5*

Tab. 42 ··· 45 see page 58

Tab. 46. $BaTiO_3$. Summary of the ESR parameters for various paramagnetic centers in doped $BaTiO_3$.

Paramagnetic center	Site	S	$\mathscr{H}$	ν GHz	T °K	g-factor	FS: D, E, a, F [10^{-2} m^{-1}]	HFS: I	HFS: A, B [10^{-2} m^{-1}]	Ref.	Literature
Mn^{2+}	Ti^{4+}	5/2	(7)	9.3	78	2.0016 ± 0.0005	$D = 56 \pm 5$	5/2	$^{55}A_{\parallel} = {}^{55}A_{\perp}$ $^{55}A_{\parallel} = 79.8 \pm 0.5$	a)	*60I1*
					300	2.0023 ± 0.0005	$D = 65 \pm 5$		$^{55}A_{\parallel} = 78.6 \pm 0.5$	b)	*63O1*
					440	2.0009 ± 0.001	$a = 14 \pm 5$		$^{55}A_{\parallel} = 79 \pm 0.5$	c)	*64I5*
	Ba^{2+}	5/2	(7)	9.3	RT	2.002 ± 0.001	$D = +(215 \pm 2)$ $E = 0$ $a = +(16.76 \pm 0.94)$		$^{55}A_{\parallel} = -(77.4 \pm 0.6)$ $^{55}A_{\perp} = -(82.3 \pm 0.8)$		
					438	2.002 ± 0.001	$D = 0$ $E = 0$ $a = +(12.11 \pm 0.94)$		$^{55}A_{\parallel} = {}^{55}A_{\perp}$ $^{55}A_{\parallel} = -(79.3 \pm 0.4)$		*66I3*[1][2]

Para-magnetic center	Site	S	$\mathscr{H}$	ν GHz	T °K	g-factor	FS D, E, a, F, b [10^{-2} m^{-1}]			HFS I	HFS A, B [10^{-2} m^{-1}]	Ref.	Literature
Fe^{3+}	Ti^{4+}	5/2	(7)	5 ··· 7.5, 10, 16.3	393, 433	2.003	$D = 0$ $a = 102 \pm 12$					d)	59H5, 62R1
				10	300	2.0036 ± 0.002	$D = +929$ $E = 0$ $a = +91 \pm 20$					e)	63S2[2])
					276	2.0036 ± 0.002	$D = -530 \pm 10$ $a = +105 \pm 20$					f)	
					213	2.0036 ± 0.002	$D = -640 \pm 10$ $E = 0 \pm 1.3$						
					77	2.0036 ± 0.002	$D = 0$ $E = 0$ $a = +115 \pm 10$						
					173	2.003 ± 0.002	$D = -23 \pm 5$ $a - F = +113 \pm 10$						64S3[2])[3])
Co^{2+}	Ti^{4+}	1/2	(3)	9	4	4.347 (isotropic)				7/2	$^{59}A_\parallel = {}^{59}A_\perp$ $^{59}A_\parallel = 109$		67Z2
							b_{20}	b_{40}	b_{60}				
Gd^{3+}	Ba^{2+}	7/2	(8)	12, 18	300	1.995 ± 0.003	−293.6 ± 1.0	+4.0 ± 1.0	1.6 ± 1.0				62R1
					425	1.995 ± 0.003	—	≈6	—				
	Ti^{4+}			10	RT	1.992	—	24 ± 0.9	−3.7 ± 2.8				64T1
					436	1.992		23.3 ± 0.4	−1.8 ± 0.4				66T3
						$g_\parallel$	$g_\perp$						
Pt^{3+}	Ti^{4+}	1/2	(3)	10	4	1.950 ± 0.005	2.459 ± 0.003			1/2	$^{195}A = 0 \pm 5$ $^{195}B = 135 \pm 5$		66S21
					78	1.935 ± 0.005	2.51 ± 0.02				$^{195}A < 28$ $^{195}B = 135 \pm 10$		63S12
Electron	oxygen vacancy	1/2	(2)	10	55	1.930	1.911					g)	63S11, 66T2, 67T3

a) Temperature dependence of D^3 in the tetragonal phase is linear. [65V4].
b) Forbidden transition lines ($\Delta M = \pm 1, \Delta m = \pm 1$) are observed. [63O1], [64I5]. Forbidden transition lines ($\Delta M = \pm 1, \Delta m = \pm 2$) are observed. [65I1], [66I3].
c) Temperature dependence of ^{55}A. [67Z1].
d) Fe^{3+} spectra are studied with a d.c. bias electric field near transition temperature from cubic to tetragonal phase and from tetragonal to orthorhombic phase. [63S3], [64E1].
e) Forbidden transition lines ($\Delta M = 2, 3, 4, 5$) are observed in the rhombohedral phase. [64S3].
f) Fe^{3+} spectra due to the oxygen vacancy; $g_\parallel \cong 2$, $g_\perp = 6.0 \pm 0.1$ at 77 °K. [65G1].
g) Hyperfine structure of an electron captured by an oxygen vacancy. [64D1].
1) Mn^{3+} ion takes the place of Ti^{4+} lattice site in ceramics, while it takes the place of Ba^{2+} in a single crystal.
2) Positive a is assumed.
3) Fe^{3+} spectra in a single-domain specimen.

Tab. 42. $BaTiO_3$, $SrTiO_3$, TiO_2, $KTaO_3$. Dispersion parameters calculated from the Kramers-Kronig analysis [*62S11*]. See Fig. 201

$$\varkappa' = \varkappa_\infty + \sum_i 4\pi \varrho_i \nu^2 \frac{\nu_i^2 - \nu^2}{(\nu_i^2 - \nu^2)^2 + \gamma_i^2 \nu^2} \qquad \varkappa'' = \sum_i 4\pi \varrho_i \nu_i^2 \frac{\gamma_i \nu}{(\nu_i^2 - \nu^2)^2 + \gamma_i^2 \nu^2}$$

	$BaTiO_3$ Ordinary ray	$SrTiO_3$	TiO_2 Ordinary ray	$KTaO_3$
$\lambda_1;\ \nu_1$	20.4; 491	18.4; 544	20.0; 500	18.2 ± 0.2; 549 ± 6
γ_1/ν_1	0.059 ± 0.002	0.049 ± 0.002	0.044 ± 0.004	0.043 ± 0.009
$4\pi\varrho_1$	0.60 ± 0.03	1.56 ± 0.06	2.0 ± 0.2	2.4 ± 0.5
$\lambda_2;\ \nu_2$	54.8; 183	56.3 ± 0.5; 178 ± 2.0	25.8; 388	49.8; 200.8
γ_2/ν_2	0.030 ± 0.006	0.039 ± 0.004	0.058 ± 0.006	0.055 ± 0.011
$4\pi\varrho_2$	2.2 ± 0.4	3.6 ± 0.4	1.08 ± 0.1	7.6 ± 1.5
$\lambda_3;\ \nu_3$	296 ± 8; 33.8 ± 0.9	114.3 ± 1.1; 87.7 ± 0.9	54.8 ± 0.5; 183 ± 1.8	107.5 ± 2.0; 93.0 ± 2.0
γ_3/ν_3	2.5 ± 0.1	0.5 ± 0.1	0.19 ± 0.01	0.5 ± 0.1
$4\pi\varrho_3$	1830 ± 70	311 ± 62	81.5 ± 4.1	163 ± 33

Resonance wavelength λ_i in 10^{-6} m; resonance frequency ν_i in $10^2\ m^{-1}$; width γ_i; strength $4\pi\varrho_i$.

Tab. 43. $BaTiO_3$, $SrTiO_3$, TiO_2. Energies of fundamental absorption edges (in eV) at RT. [*65C2*]

	E_0	A_1	A_2	A_3	B_1	B_2	C_1	C_2	D	E	
$SrTiO_3$	3.2	4.00	4.86	5.5	6.52	7.4	9.2	9.9	12.5	15.3	eV
$BaTiO_3$	3.2	3.91	4.85		6.10	7.25	10.3	11.8	12.8	15	eV
TiO_2 ($E \perp c$)		3.97	5.52		6.50	7.64	8.53	9.24	11	14.1	eV

Tab. 44. $BaTiO_3$, $SrTiO_3$, $KTaO_3$, $KTa_{0.35}Nb_{0.65}O_3$ (KTN), TiO_2. Band gap energies $\hbar\omega_g$ (in eV). [*67B1*]. See Fig. 46, 103, 216, 430. F_1, F_2: different dispersion functions $F_i(\omega/\omega_g)$, see [*67B1*]

	$SrTiO_3$		$BaTiO_3$	$KTaO_3$		KTN	TiO_2	
	296 °K	77 °K	403 °K	296 °K	77 °K	296 °K	296 °K	
Faraday rotation $\hbar\omega_g$ for F_1	3.40	3.43	3.25	3.77	3.79	3.54	3.62	eV
Faraday rotation $\hbar\omega_g$ for F_2	3.21	3.26	3.11	3.62	3.65	3.36	3.37	eV
Energy of reflectivity peak or shoulder	3.20	—	3.20	—	—	3.70	—	eV
Energy of electroreflectance singularity	—	—	3.20	3.57 3.80	—	3.60	3.00 3.30	eV eV
$\hbar\omega_g$ from absorption data	3.40	—	—	3.75	—	—	—	eV
Energy at which absorption coefficient $\alpha \approx 10^4\ cm^{-1}$	3.37	—	3.26	3.79	—	3.45	3.18	eV

Tab. 45. $BaTiO_3$ (reduced or doped). List of reference papers on PTC anomaly

Materials (dopants)	References	Materials (dopants)	References
Single crystal		Ceramics	
$BaTiO_3$: reduced	*57H1, 63K3, 64I4, 64G4, 65M1, 65U2*	$BaTiO_3$	*63H5, 65U2*
$BaTiO_3$: Nb	*64B11*	$BaTiO_3$: La	*59S1, 63T3, 64J1, 65M1*
		$BaTiO_3$: Ce	*63T3*
		$BaTiO_3$: Sm	*63G5*
		$BaTiO_3$: Gd	*65U2*
		$BaTiO_3$: Sb	*65A3*
		(Ba-Sr)TiO_3	*61H5, 65A3*
		(Ba-Sr)TiO_3: La	*59S1, 61T1, 63T3*
		$BaTiO_3$: Sr, Ce, Sn	*61S1*
		$BaTiO_3$: Sr, Ca, Sn	*61S1*
		$BaTiO_3$: Sr, Bi	*63T3*
		$BaTiO_3$: Mg, Ce	*61S1*
		$BaTiO_3$: Zr, Ce	*61S1*
		$BaTiO_3$: Si, Ce	*61S1*

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Nr. 1A-9 $PbTiO_3$, Lead titanate

1a	Ferroelectric activity was reported independently by SHIRANE et al. and by SMOLENSKII in 1950.	*50S4* *50S6*
b	see table below	a) *51S6* b) *55K3* c) *46M2*
	$a = 3.904_5$ Å, $c = 4.152_4$ Å at RT (in phase II).	*46M2*
2a	Crystal growth: KF flux method; $PbCl_2$ flux method.	*58K1, 52N2*
b	Crystal form: Fig. 271.	
3	Crystal structure: Positional parameters: Tab. 47, 48. Projection of crystal structure: Fig. 272, 273.	
4	Thermal expansion: Fig. 274 ··· 280. Dependence of lattice parameters on hydrostatic pressure: Fig. 281.	
5a	Dielectric constants: Fig. 282. Small dielectric anomaly was observed at about −100 and −150 °C.	*56K2*
	Curie-Weiss constant: $C = 1.1 \cdot 10^5$ °K (single crystal).	*62B4*
6a	Specific heat: Fig. 283.	
	see table below	*51S7* *51S7*
c	Thermal conductivity: Fig. 284.	
7a	Piezoelectric properties: Tab. 49.	
9a	Birefringence: Fig. 285. Infrared absorption: Fig. 286, 287. Frequencies of infrared modes: Tab. 50.	
12b	ESR: Tab. 51.	
14a	Domain structures were observed by polarized light.	*52N2, 58K1, 59K1*
16	Radiation damage: Fig. 288.	

1b:

phase	III[b])*	II[a])	I[a])	
state		F[a])	P[a])	
crystal system		tetragonal[c])	cubic[a])	
space group		P4mm-C^1_{4v}	Pm3m-O^1_h	
Θ	−100[b])		490[a])	°C

6a:

	II−I	
ΔQ_m	1150	cal mol^{-1}
ΔS_m	1.6	cal °K^{-1} mol^{-1}

Tab. 47. $PbTiO_3$. Positional parameters of atoms at RT. [*56S5*]

	x	y	z
Pb	0	0	0
Ti	½	½	0.540
O(1)	½	½	0.112
O(2)	½	0	0.612
	0	½	0.612

Tab. 48. $PbTiO_3$. Bond lengths in Å at RT (phase II) and at 490 °C (phase I) [*56S5*]. $O(1)_+$ represents the O(1) ion closer to, $O(1)_-$ that further away from Ti. Similarly $O(2)_+$ is closer to Pb

phase	II (at RT)	I (at 490 °C)
Ti-$O(1)_+$	1.78	1.89
Ti-$O(1)_-$	2.38	
Ti-O(2)	1.98	
Pb-O(1)	2.80	2.80
Pb-$O(2)_+$	2.53	
Pb-$O(2)_-$	3.20	

* Phase transition II-III was reported to occur only if the cooling rate is extremely slow. [*55K3*]

Tab. 49. $PbTiO_3$ (modified ceramics). Electromechanical constants at RT. [68U1]

Additive	$PbNb_{4/5}O_3$ 5.0 mol%	$BiZn_{1/2}Ti_{1/2}O_3$ 5.0 mol%	$Bi_{2/3}Zn_{1/3}Nb_{2/3}O_3$ 5.0 mol%	
a	3.915	3.904	3.911	Å
c	4.104	4.148	4.133	Å
c/a	1.049	1.062	1.057	
ϱ	7.19	7.68	7.12	10^3 kg m^{-3}
porosity	0.105	0.036	0.10	
Θ	466	524	494	°C
$\varkappa^T_{11}$	—	195	244	
$\varkappa^T_{33}$	226	147	203	
d_{31}	10	3.9	7.4	10^{-12} C N^{-1}
d_{33}	37	37	47	10^{-12} C N^{-1}
g_{31}	5.2	3.0	4.1	10^{-3} m^2 C^{-1}
g_{33}	16	28	28	10^{-3} m^2 C^{-1}
s^E_{11}	1.2	1.2	1.1	10^{-11} m^2 N^{-1}
s^E_{33}	1.1	0.95	1.1	10^{-11} m^2 N^{-1}
Q_{mech}				
for s_{11}	336	54	326	
for s_{33}	71	74	76	
k_{15}	—	0.40	0.36	
k_{31}	0.068	0.031	0.052	
k_{33}	0.23	0.32	0.35	

Tab. 50. $PbTiO_3$. Wave numbers in 10^2 m^{-1} and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Ti-O stretch)	$\tilde{\nu}_2$ (Ti-O_3 torsion)	$\tilde{\nu}_3$ (O-Ti-O bend)	$\tilde{\nu}_4$ (cation-TiO_3 lattice mode)
530 (E_u, A_1)	400 (B_1, E_u)	220 (E_u, A_1) 172	83 (E_u, A_1)

Tab. 51. $PbTiO_3$. g-factors at RT. [64G1]

Paramagnetic center	Site	S	$\mathscr{H}$	ν GHz	T °K	g-factor	
						$g_\parallel$	$g_\perp$
Fe^{3+}	Ti^{4+}	1/2*	(2)	8.8	RT	2.009 ± 0.005	5.97 ± 0.02

The spectrum up to 300 °C and down to −120 °C did not show any fundamental change.

Nr. 1A-10 $CaZrO_3$, Calcium zirconate

1	A few physical properties of $CaZrO_3$ were studied in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be orthorhombic with the cell dimensions $a = 5.587$ Å, $b = 8.008$ Å, $c = 5.758$ Å at RT.	*55C1*
4	Linear thermal expansion: $\alpha = 8.55 \cdot 10^{-6}$ °C^{-1} between 23 °C and 223 °C; $\alpha = 9.53 \cdot 10^{-6}$ °C^{-1} between 223 °C and 333 °C for ceramics of bulk density $\varrho = 4.95 \cdot 10^3$ kg m^{-3}	*65B10*
9	Infrared absorption: Fig. 289, 290; Tab. 52.	

Tab. 52. $CaZrO_3$. Wave numbers in 10^2 m^{-1} and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O_3 torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO_3 lattice mode)
515 (B_1, B_2, A_1)	340 (B_1, B_2, A_2) (377) (418)	228 (B_1, B_2, A_1) 186	153 (B_1, B_2, A_1) 96

* The ficticious spin is ½ [64G1].

Nr. 1A-11 $SrZrO_3$, Strontium zirconate

1	A few physical properties of $SrZrO_3$ were studied in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be pseudo-cubic with $a' = 4.099$ Å at RT.	*57R2*
4	Linear thermal expansion: $\alpha = 8.75 \cdot 10^{-6}$ °C^{-1} between 23 °C and 320 °C; $\alpha = 9.34 \cdot 10^{-6}$ °C^{-1} between 320 °C and 700 °C for ceramics of bulk density $\varrho = 5.00 \cdot 10^3$ kg m^{-3}.	*65B10*
9	Infrared absorption: Fig. 291, 292; Tab. 53.	

Tab. 53. $SrZrO_3$. Wave numbers in 10^2 m^{-1} and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [*65P4*]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O_3 torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO_3 lattice mode)
522 (B_1, B_2, A_1)	325 (B_1, B_2, A_2) (357) (379)	240 (B_1, B_2, A_1)	143 (B_1, B_2, A_1)

Nr. 1A-12 $BaZrO_3$, Barium zirconate

1	A few properties of $BaZrO_3$ were reported in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be cubic with the cell dimensions $a = 4.192$ Å at RT.	*57R2*
4	Linear thermal expansion: $\alpha = 5.64 \cdot 10^{-6}$ °C^{-1} between 23 °C and 214 °C; $\alpha = 6.54 \cdot 10^{-6}$ °C^{-1} between 214 °C and 324 °C for ceramics of bulk density $\varrho = 6.73 \cdot 10^3$ kg m^{-3}.	*65B10*
9	Infrared absorption: Fig. 293, 294; Tab. 54.	

Tab. 54. $BaZrO_3$. Wave numbers in 10^2 m^{-1} and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [*65P4*]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O_3 torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO_3) lattice mode)
505 (F_{1u})	– (F_{2u})	210 (F_{1u})	115 (F_{1u})

Nr. 1A-13 $PbZrO_3$, Lead zirconate

1a Dielectric anomaly of $PbZrO_3$ associated with a phase transition was reported independently by Roberт and by Smolenskii in 1950. Antiparallel ionic shifts on the (001) projection of crystal structure were found by Sawaguchi et al. in 1951. In the same year antiferroelectric double hysteresis loops were discovered by Shirane et al.. $PbZrO_3$ is the first compound in which double hysteresis loops were observed. — *50R1*, *50S7*, *51S3*, *51S8*

b.

phase	II[a])	I[a])
state	A[b])	P[a])
crystal system	orthorhombic[c])	cubic[c])
space group	Pba2-C_{2v}^8 [c])	Pm3m-O_h^1 [c])
Θ	230 °C[a])	

[a]) *50R1*
[b]) *51S8*
[c]) *51S3*

$a = 5.87$ Å, $b = 11.74$ Å, $c = 8.20$ Å at RT (in phase II). The cubic unit cell in phase I becomes pseudo-tetragonal in phase II. The pseudo-tetragonal cell constants a' and c' are related with the orthorhombic cell constants a, b and c: $a = \sqrt{2}\,a'$, $b = 2\sqrt{2}\,a'$ and $c = 2c'$, where $a' = 4.15$ Å, $c' = 4.10$ Å at RT. Relation between the pseudo-tetragonal and orthorhombic cells: Fig. 295. — *51S3*

2a Crystal growth: $PbCl_2$ flux method. — *55J2*

	Nr. 1A-13 $PbZrO_3$ continued	
3	$Z = 8$ (in phase II). The crystal is polar along the c axis and antipolar along the a axis in phase II. Fig. 295 shows schematically the shifts of Pb ions. Positional parameters and shifts from ideal perovskite positions: Tab. 55. Projection of ZrO_6: Fig. 296, 297, 298. Bond distances between Zr and O: Fig. 299.	51S3, 57J4, 51S3 57J4
4	Thermal expansion: Fig. 300 ··· 303. $\alpha_{a'} \cong -0.05 \cdot 10^{-5}$ °K^{-1} and $\alpha_{c'} \cong 2.80 \cdot 10^{-5}$ °K^{-1} in phase II; $\alpha_{a'} \cong 1.10 \cdot 10^{-5}$ °K^{-1} in phase I, where $\alpha_{a'}$ and $\alpha_{c'}$ are the linear thermal expansion coefficients along the pseudo-tetragonal a' and c' axes, respectively.	52S1
5a	Dielectric constants: Fig. 304. $C = 1.36 \cdot 10^5$ °K (determined with ceramics). Effect of pressure: Fig. 305. $(d\Theta_a/dp)_{p\to 0} = (4.1 \pm 0.2)\ 10^{-8}$ °K N^{-1} m^2.	50R1
c	Critical field: Fig. 306.	66R2
6a	Specific heat: Fig. 307. For the transition II-I: $\Delta Q_m = 440$ cal mol^{-1}; $\Delta S_m = 0.88$ cal °K^{-1} mol^{-1}.	52S2
b	Thermal conductivity: Fig. 308.	
8	Elastic compliances: Fig. 309.	
9a	Birefringence: Fig. 310. Infrared absorption: Fig. 311, 312; Tab. 56.	
16	Radiation damage: Fig. 313.	

Tab. 55. $PbZrO_3$ (ceramics). Atomic coordinates and shifts from ideal perovskite positions at RT. [57J4]

Atom	x	y	z	Wyckoff notation	Total shift Å
Pb'	0.706	0.127	0	4c	0.26
Pb"	0.706	0.127	0.500	4c	0.26
Zr'	0.243	0.124	0.250	4c	0.04
Zr"	0.243	0.124	0.250	4c	0.04
O(1)'	0.270	0.150	0.980	4c	0.35
O(1)"	0.270	0.100	0.480	4c	0.35
O(2)'	0.040	0.270	0.300	4c	0.53
O(2)"	0.040	0.270	0.750	4c	0.34
O(3)'	0	0.500	0.250	2b	0
O(3)"	0	0.500	0.800	2b	0.41
O(4)'	0	0	0.250	2a	0
O(4)"	0	0	0.800	2a	0.41

Tab. 56. $PbZrO_3$. Wave numbers in 10^2 m^{-1} and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O_3 torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO_3 lattice mode)
508 (E_u, A_1)	290 (B_1, E_u)	221 (E_u, A_1)	80 (E_u, A_1) 34

Nr. 1A-14 $PbHfO_3$, Lead hafnate

1a	A dielectric anomaly associated with a phase transition was observed, and the possibility of the antiferroelectricity was discussed by Shirane et al. in 1953.				53S3
b	phase	III	II	I	53S3
	state	(A)		P	
	crystal system	pseudo-tetragonal	tetragonal	cubic	
	Θ	163	215	°C	
	Lattice constants for the pseudo-tetragonal phase: $a' = 4.136$ Å, $c'/a' = 0.991$ at RT.				53S3

4	Thermal expansion: Fig. 314. Cubic thermal expansion coefficients: below 158 °C: $20 \cdot 10^{-6}\ deg^{-1}$; above 215 °C: $27 \cdot 10^{-6}\ deg^{-1}$.	*53S3*
5a	Dielectric constant: Fig. 315. $C = 9.5 \cdot 10^4$ °K (ceramics).	*53S3*

Nr. 1A-15 $BiFeO_3$, Bismuth ferrite

1a In 1960[a]) it was pointed out on the basis of x-ray studies of the solid solution, $PbTiO_3$-$BiFeO_3$, that $BiFeO_3$ could have a ferroelectric Curie point at high temperatures. The Curie point was estimated to be about 850 °C from studies of the same solid solution[b]).
Disagreement, however, exists among many experimental data reported so far, therefore reservation is necessary in deciding whether $BiFeO_3$ is ferroelectric or antiferroelectric.
Antiferromagnetic anomaly in $BiFeO_3$ was observed by direct magnetic measurements at about 370 °C[c]).

[a]) *60F9, 60V2*
[b]) *61F3, 62F8*
[c]) *62S10, 63R1, 65I2*

b

phase	IV		III		II		I	
state	(A) or (F), A^{*}_{magn}		(A) or (F), P_{magn}		(A) or (F), P_{magn}		(P), P_{magn}	
crystal system	rhombohedral		rhombohedral		rhombohedral		cubic (possibly)	
space group	R3m-C^{5}_{3v}**							
Θ		370		≈575		850		°C

$a = (3.962 \pm 0.001)$ Å, $\alpha = 89°\ 31' \pm 3'$ at RT. — *64T6*
Further references are available on unit cell parameters. — *60V2, 60F6, 60Z2*

3 Crystal structure: From the x-ray diffraction studies, $BiFeO_3$ was found to belong to one of the five space groups: R 3, R $\bar{3}$, R 32, R3m and R$\bar{3}$m. — *60Z2*
Neutron diffraction studies suggested that $BiFeO_3$ belongs to the non-centrosymmetric space group R3m. The crystal structure can be regarded as consisting of alternating FeO_3 and BiO_3 trigonal pyramids: Fig. 316; Tab. 57. — *63K5*
According to the electron diffraction study, $BiFeO_3$ belongs to the non-centrosymmetric space group R3m at RT. Atomic coordinates: Tab. 58. — *64T6*
The space group R3m was, however, rejected by Smolenskii et al., because it does not satisfy the conditions for the existence of weak ferromagnetism. — *64S9*
The magnetic structure of $BiFeO_3$ was proved to be G-type by the neutron diffraction experiments. Fig. 317, 318. — *63K5*

4	Unit cell parameters: Fig. 319, 320. See also	*66R8, 64T5*
5a	Dielectric constant: Fig. 321, 322, 323. No reliable data on the dielectric constant in the high temperature region near 850 °C are available.	
11	Magnetic susceptibility: Fig. 324. At RT, no spontaneous magnetic moment was observed in the fields up to 22 kOe.	
12c	Mössbauer effect: Fig. 325, 326.	
17	Calculations of the internal electric fields and their gradients in $BiFeO_3$ crystals were made on the basis of an ionic model.	*67T7*

Tab. 57. $BiFeO_3$. Values of the interatomic distances [Å]. [*63K5*]. See Fig. 316. See also [*64T6*]

	520 °C	20 °C
Bi-Fe (*A*)	3.841	3.857
Bi-Fe (*B*)	3.006	2.994
Bi-O (*C*)	2.903	2.907
Bi-O (*D*)	2.680	2.693
Fe-O (*F*)	2.233	2.214
Fe-O (*G*)	1.754	1.774
O-O (*H*)	2.841	2.859
O-O (*K*)	2.800	2.800
O-O (*L*)	2.680	2.724

Tab. 58. $BiFeO_3$. Atomic coordinates. [*64T6*]

Atom	*x*	*y*	*z*
Bi	0.0337	0.0337	0.0337
Fe	0.5000	0.5000	0.5000
O(1)	−0.0280	0.5000	0.5000
O(2)	0.5000	−0.0280	0.5000
O(3)	0.5000	0.5000	−0.0280

* This state is presumably weak ferromagnetic. [*66Y2*]
** See subsection 3.

Nr. 1A-16 KIO_3, Potassium iodate

1a Ferroelectric behavior in KIO_3 was reported by Herlach in 1961. — 61H3

b

phase	V[a]	IV[a]	III[a]	II[a]	I[a]
state		F[a]	F[a]	F[a]	P[a]
crystal system			trigonal[b]*		trigonal[a]
Θ	−190[a]	−18, −10[a]**	70[a]	212[a]	°C

[a]) 61H3; [b]) 60S5

$T_{melt} = 560$ °C. — 66H17

$\varrho = 3.979$[1]) $\cdot 10^3$ kg m^{-3}. — 08g1

[1]) A different value, 3.802, is also given in the same reference.

$a = (4.410 \pm 0.005)$ Å $\alpha = 89{,}41°$ at RT, adopting trigonal system. — 60S5

$a = 8.921$ Å, $b = 8.916$ Å, $c = 8.885$ Å, $\alpha \cong \beta \cong \gamma \cong 90° \pm 30'$ at RT, adopting triclinic system. — 65F3

Transparent

2a Hydrothermal method: Fig. 327. — 61H3

Growth from the supersaturated solution with $10 \cdots 14\%$ HIO_3 at a constant temperature: Fig. 328. — 27m1

3 $Z = 1$ in phase III, adopting trigonal system. — 61H3

$Z = 8$ in phase III, adopting triclinic system. — 65F3

4 Lattice deformation: $a = [4.44 + 0.00022\ (T - 220)]$ Å, $\alpha = 89°\,20' - 0.09\ (T - 220)'$ in phase I (T in °C). — 61H3

5a Dielectric constants: Fig. 329, 330. — 66H17

c Spontaneous polarization: Fig. 331. — 61H3

9a Absorption edge: Fig. 332. — 67V2

12a NMR: Fig. 333. — 61H3

1B Complex perovskite-type oxides

Nr. 1B1-i $(K_{1/2}Bi_{1/2})TiO_3$, Potassium bismuth titanate

1a Ferroelectricity in $(K_{1/2}Bi_{1/2})TiO_3$ was found by Smolenskii and Agranovskaya in 1959. — 59S6

b

phase	III	II	I
state	(F)	(A)	P
crystal system	tetragonal	pseudo-cubic	cubic
space group			$Pm3m\text{-}O_h^1$
Θ	270	410,380[a])	°C

62I5; [a]) 60S6

$a = (3.913 \pm 0.003)$ Å, $c = (3.993 \pm 0.003)$ Å at RT.

3 Crystal structure: Disordered perovskite. — 62I5

4 Lattice distortion: Fig. 334.

Thermal expansion: Fig. 335.

5a Dielectric constant: Fig. 336.

Nr. 1B1-ii $(Na_{1/2}Bi_{1/2})TiO_3$, Sodium bismuth titanate

1a Ferroelectricity in $(Na_{1/2}Bi_{1/2})TiO_3$ was found by Smolenskii and Agranovskaya in 1959. — 59S6

* Various crystal systems have been proposed: trigonal [*60S5*], triclinic [*65F3*].

** −10 °C on heating, −18 °C on cooling.

1b	phase	III	II	I	
	state	F	(A)	P	
	crystal system	rhombohedral	pseudo-cubic	cubic	*62I5*
	space group			Pm3m-O_h^1	
	Θ		≈200[a])	320 °C	[a])*60S6*

	$a = (3.891 \pm 0.002)$ Å, $\alpha = 89° 36' \pm 3'$ at RT.	
3	Crystal structure: Disordered perovskite.	*62I5*
4	Thermal expansion: Fig. 337.	
5a	Dielectric constant: Fig. 338.	
c	Spontaneous polarization and coercive field: $P_s \approx 8.0 \cdot 10^{-2}$ C m^{-2}; $E_c \approx 14 \cdot 10^2$ kV m^{-1} at 116 °C.	*60S6*

Nr. 1B2-i $Pb(Mg_{1/2}W_{1/2})O_3$

1a	Antiferroelectric properties of $Pb(Mg_{1/2}W_{1/2})O_3$ were discovered by Smolenskii et al. in 1959.	*59S7*

b	phase	II	I	
	state	A	P	
	crystal system	orthorhombic	cubic	*62Z1*
	space group	C222$_1$-D_2^5		
	Θ	38 °C		

	$a = 22.74$ Å, $b = 22.79$ Å, $c = 15.90$ Å at RT. Orthorhombic unit cell: see Fig. 339.	
2a	Crystal growth: Crystal growth of $Pb(Mg_{1/2}W_{1/2})O_3$ was reported by Myl'nikova.	*60M2*
3	Crystal structure: $Pb(Mg_{1/2}W_{1/2})O_3$ has the structure of perovskite type. Fig. 339. $Z = 64$ (molecular unit: Pb_2MgWO_6).	*62Z1*
4	Lattice distortion associated with the phase transition. Thermal expansion: Fig. 340.	*62Z1*
5a	Dielectric constants: Fig. 341, 342, 343. $d\Theta_a/dp = -5.84 \cdot 10^8$ °K N^{-1}m^2.	
6	Specific heat: Fig. 344. Transition heat (II → I): $\Delta Q_m = 276$ cal mol^{-1}.	*66S28*
8a	Elastic compliance: Fig. 345. Ultrasound absorption: Fig. 346, 347.	

Nr. 1B2-ii $Pb(Cd_{1/2}W_{1/2})O_3$

1a	Synthesis of $Pb(Cd_{1/2}W_{1/2})O_3$ was reported by Belyaev et al. in 1963.	*63B3*

b	phase	II	I	
	state	(A)	P	
	crystal system	monoclinic	cubic	
	Θ	400 °C		*65F4*

	$a = (4.156 \pm 0.002)$ Å, $b = (4.074 \pm 0.002)$ Å, $\beta = 91° 9' \pm 5'$ at RT. Roginskaya and Venevtsev reported that another transition exists at 120 °C, in addition to the transition at 400 °C.	*65R4*
3	Crystal structure: Superstructure lines, indicating ordered location of the octahedral voids of the perovskite lattice, were observed.	*65F4*
4	Lattice distortion: Fig. 348, 349.	
5a	Dielectric constant: Fig. 350.	

Nr. 1B2-iii $Pb(Mn_{1/2}W_{1/2})O_3$

1a A synthesis of $Pb(Mn_{1/2}W_{1/2})O_3$ was reported by Venevtsev et al. — *64V3*

b

phase	II	I	
state	(A), P_{magn}	P, P_{magn}	
crystal system	monoclinic	cubic	
Θ		423	°K

$a = 4.063$ Å, $b = 4.033$ Å, $\beta = 90° 12'$ at RT. — *65R5*

5a Dielectric constant: Fig. 351. — *65R5*

10 Electrical conductivity: $\sigma = 8 \cdot 10^{-8}\ \Omega^{-1}\ m^{-1}$. — *65R5*

11 Magnetic susceptibility: see Fig. 351.

Nr. 1B2-iv $Pb(Co_{1/2}W_{1/2})O_3$

1a Antiferro- and ferroelectric properties in $Pb(Co_{1/2}W_{1/2})O_3$ were discovered by Filip'ev et al. — *63F1*

b — *65B8*, [a]*66K6*, [b]*64F4*

phase	IV	III	II	I	
state	F, F_{magn} (weak)	F, P_{magn}	A, P_{magn}	P, P_{magn}	
crystal system			orthorhombic	cubic	
Θ	9[a]	83 ··· 103	293[b] 305		°K

$a = 4.008$ Å at 298 °K.

2a Crystal growth: Flux method with PbO. — *65B8*

3 Crystal structure: A superstructure was observed which was completely explained by alternation of the population of the oxygen octahedra by Co^{2+} and W^{6+} cations along the three directions. The real elementary lattice is a cubic face centered one with the parameter $A = 2a$ for phase I and with the parameters $A = 2\cos(\beta/2)$, $B = 2b$, and $C = 2a\sin(\beta/2)$ for II, where a, b and β are the parameters of the perovskite sub-lattice. — *64F4*

4

phase	lattice parameters
I	$A = 8.017$ Å at 298 °K
II	$A = 5.669$ Å, $B = 7.956$ Å, $C = 5.689$ Å at 258 °K

Lattice distortion: Fig. 352. — *64F4*

5a Dielectric constant: Fig. 353, 354, 355.

c Polarization: Fig. 356.

11 Magnetic susceptibility and magnetization: Fig. 357, 358.

Nr. 1B2-v $Pb(Mn_{1/2}Re_{1/2})O_3$

1a A synthesis of $Pb(Mn_{1/2}Re_{1/2})O_3$ was reported by Venevtsev et al. — *64V3*

b

phase	III	II	I	
state	(A), F_{magn}	(A), P_{magn}	P, P_{magn}	
crystal system		monoclinic	cubic	
Θ	103	393		°K

$a = 4.043$ Å, $b = 4.012$ Å, $\beta = 90° 33'$ at RT. — *65R5*

3 Crystal structure: Ordered perovskite. — *65R5*

4	Lattice distortion: Fig. 359.	*65R5*
10	Electrical conductivity: $\sigma = 1 \cdot 10^{-1}\,\Omega^{-1}\,m^{-1}$.	*65R5*
11	Magnetic susceptibility and magnetic moment: Fig. 360. The linear temperature dependence of χ^{-1}_{magn} with a positive value of $\Theta_{p\,magn} = 85$ °K, and the appearing of the spontaneous moment at 103 °K, may indicate the presence of ferromagnetic properties in this compound, which is in agreement with the positive sign of the indirect exchange interaction proposed by GOODENOUGH for Mn^{2+} and Re^{6+} ions. However, the magnitudes of the calculated theoretical spontaneous moments agree with the experimental values only on the assumption of an antiferromagnetic interaction between ions distributed in an ordered fashion over the octahedral vacancies.	*65R5*

Nr. 1B3-i $Pb(Sc_{1/2}Nb_{1/2})O_3$

1a	Ferroelectricity in $Pb(Sc_{1/2}Nb_{1/2})O_3$ was discovered by SMOLENSKII et al. in 1959.	*59S9*
b	(see table below)	*59S9*; [a]) *60I3*

phase	II	I
state	F	P
crystal system	tetragonal[a]) (possibly)	cubic
Θ	90 °C	

$a = (4.074 \pm 0.001)$ Å, $c = (4.083 \pm 0.001)$ Å at RT.[a])

3	Crystal structure: In the powder patterns, additional to the principal lines of the perovskite structure, superstructural lines were observed indicating a doubling of the lattice period.	*59I3*
5a	Dielectric constant: Fig. 361.	
c	Spontaneous polarization: $P_s \approx 3.6 \cdot 10^{-2}\,cm^{-2}$ at 18 °C.	*59S9*

Nr. 1B3-ii $Pb(Mn_{1/2}Nb_{1/2})O_3$

1a	A synthesis of $Pb(Mn_{1/2}Nb_{1/2})O_3$ with perovskite structure was reported by VENEVTSEV et al.	*64V3*

Nr. 1B3-iii $Pb(Fe_{1/2}Nb_{1/2})O_3$

1a	Ferroelectricity in $Pb(Fe_{1/2}Nb_{1/2})O_3$ was discovered by SMOLENSKII et al. in 1958.	*58S4*
b	(see table below)	*62B7*, *64S8*, *62B10*

phase	III	II	I
state	F, A_{magn}	F, P_{magn}	P, P_{magn}
crystal system	rhombohedral	rhombohedral	cubic
space group			$Pm3m\text{-}O_h^1$
Θ	143 °K	387 °K	

$a = 4.014$ Å, $\alpha = 89.92°$ at RT.

2a	Crystal growth: Flux method with PbO.	*62B7*
3	Crystal structure: Disordered perovskite; X-ray studies have not shown any ionic ordering in the octahedral sites of perovskite structure. The magnetic peak was found in the neutron diffraction experiments at 78 °K. The effective magnetic moment of the Fe^{3+} ion was found to be $(0.80 \pm 0.16)\,\mu_B$ at 78 °K from the calculation of the intensity of the (111) reflection, which is about 90% of the magnetic moment at 0 °K. Fig. 362.	*64S8* *65D6*
5a	Dielectric constant: Fig. 363.	
9a	Optical absorption: Fig. 364.	
11	Magnetic susceptibility: Fig. 365. $\mu_{eff} = 5.4\,\mu_B$.	*62B7*
12b	ESR: Fig. 366.	
c	Mössbauer effect: Fig. 367, 368. The quadrupile splitting $\Delta E_{qu} = (0.37 \pm 0.02)$ mm sec^{-1}, the isomer shift $\delta = (0.52 \pm 0.02)$ mm sec^{-1}, corresponding to trivalent iron (at 20 °C).	*66S22*

Nr. 1B3-iv $Pb(Co_{1/2}Nb_{1/2})O_3$

1a	A synthesis of $Pb(Co_{1/2}Nb_{1/2})O_3$ with perovskite structure was reported by Venevtsev et al.	*64V3*
b	Informations on the dielectric and magnetic properties are available:	*65R5*

Nr. 1B3-v $Pb(Ni_{1/2}Nb_{1/2})O_3$

1a	$Pb(Ni_{1/2}Nb_{1/2})O_3$ with perovskite structure was synthesized by the addition of 5 mol % BaO.	*65S17*

Nr. 1B3-vi $Pb(In_{1/2}Nb_{1/2})O_3$

1a	Dielectric anomaly in $Pb(In_{1/2}Nb_{1/2})O_3$ was found by Kupriyanov and Fesenko in 1965.	*65K9*
b	(table below)	*65K9*
5a	Dielectric constant: Fig. 369.	

phase	II	I
state	(F)	P
crystal system	monoclinic (possibly)	cubic
Θ	90	°C

$a = 4.11$ Å at RT.

Nr. 1B3-vii $Pb(Yb_{1/2}Nb_{1/2})O_3$

1a	Antiferroelectric properties in $Pb(Yb_{1/2}Nb_{1/2})O_3$ were reported by Filip'ev et al. in 1963.	*63F1*
b	(table below)	*65K9*, [a])*64T4*
3	Crystal structure: Superstructure lines, corresponding to ordering of Yb^{3+} and Nb^{5+} ions were found.	*64T4*
4	Lattice distortion: Fig. 370. Thermal expansion: Fig. 371.	
5a	Dielectric constant: Fig. 372.	

phase	II	I
state	AF	P
crystal system	monoclinic	cubic
Θ	300, 310[a])	°C

$a = 4.168$ Å, $b = 4.107$ Å, $\beta = 90°\,27'$ at RT[a]).

Nr. 1B3-viii $Pb(Ho_{1/2}Nb_{1/2})O_3$

1a	Dielectric anomaly in $Pb(Ho_{1/2}Nb_{1/2})O_3$ was found by Kupriyanov and Fesenco.	*65K9*
b	(table below)	*65K9*
5a	Dielectric constant: Fig. 373.	

phase	II	I
state	(A)	P
crystal system	monoclinic	cubic
Θ	240	°C

$a = 4.160$ Å, $b = 4.106$ Å, $\beta = 90°\,30'$ at RT.

Nr. 1B3-ix $Pb(Lu_{1/2}Nb_{1/2})O_3$

1a	Dielectric anomaly in $Pb(Lu_{1/2}Nb_{1/2})O_3$ was found by Smolenskii and Agranovskaya in 1958.	*58S3*

1b	phase	II	I	65K9
	state	(A)	P	
	crystal system	monoclinic	cubic	
	Θ	270 °C		
	$a = 4.152$ Å, $b = 4.093$ Å, $\beta = 90°\ 30'$ at RT.			
4	Thermal expansion: Fig. 374.			
5a	Dielectric constant: Fig. 375.			

Nr. 1B3-x $Pb(Sc_{1/2}Ta_{1/2})O_3$

1a	Ferroelectricity in $Pb(Sc_{1/2}Ta_{1/2})O_3$ was discussed by Smolenskii et al. in 1959.			59S9
b	phase	II	I	59S9
	state	F	P	
	crystal system	tetragonal[a]) (possibly)	cubic	[a])59I3
	Θ	26 °C		
	$a = (4.072 \pm 0.001)$ Å, $c = (4.072 \pm 0.001)$ Å at RT[a]).			
3	Crystal structure: The large number of superstructure lines and their great intensity in $Pb(Sc_{1/2}Ta_{1/2})O_3$ indicates that the degree of ordering of Sc^{3+} and Ta^{5+} ions is greater than in $Pb(Sc_{1/2}Nb_{1/2})O_3$. See 1B3-i-3.			59I3
5a	Dielectric constant: Fig. 376.			

Nr. 1B3-xi $Pb(Mn_{1/2}Ta_{1/2})O_3$

1a	$Pb(Mn_{1/2}Ta_{1/2})O_3$ with perovskite structure was synthesized by the addition of 5 mol% SrO.	65S17

Nr. 1B3-xii $Pb(Fe_{1/2}Ta_{1/2})O_3$

1a	Ferroelectricity in $Pb(Fe_{1/2}Ta_{1/2})O_3$ was discovered by Smolenskii et al. in 1959.				59S7
b	phase	III	II	I	68N1 [a])65S17
	state	F, A_{magn}	F, P_{magn}	P, P_{magn}	
	crystal system	rhombohedral	rhombohedral[a])	cubic	
	space group			$Pm3m\text{-}O_h^1$	
	Θ	143, 133[a])	243, 233[a]) °K		
	$P_s \parallel [111]$ (probably). $a = (4.007 \pm 0.001)$ Å at RT. black (dark orange for thin samples).				
2a	Crystal growth: Flux method with PbO. When the soak temperature is higher than 1200 °C, crystals are obtained having both pyrochloride and perovskite structure.				68N1
3	Crystal structure: Disordered perovskite.				65S17
4	phase	lattice constants			68N1
	I	$a = (4.007 \pm 0.001)$ Å at RT.			
	II	$a = (4.006 \pm 0.001)$ Å at 90 °K $\alpha = 89.89° \pm 0.02°$			
5a	Dielectric constant: Fig. 377, 378.				
c	Spontaneous polarization: Fig. 379.				
11	Magnetic susceptibility: Fig. 380. $\mu_{eff} = 5.92\ \mu_B$; $\Theta_{p\,magn} = -370$ °K.				68N1

Nr. 1B3-xiii $Pb(Co_{1/2}Ta_{1/2})O_3$

1a A synthesis of $Pb(Co_{1/2}Ta_{1/2})O_3$ with perovskite structure was reported by Shvorneva and Venevtsev. The compound was stabilized by the addition of 1 mol% La_2O_3. *65S17*

Nr. 1B3-xiv $Pb(Yb_{1/2}Ta_{1/2})O_3$

1a Dielectric anomaly in $Pb(Yb_{1/2}Ta_{1/2})O_3$ was reported by Isupov and Kranik in 1964. *64I6*

b

phase	II	I
state	(A)	F
crystal system	monoclinic	cubic
Θ	280, 285[a])	°C

$a = 4.154$ Å, $b = 4.108$ Å, $\beta = 90°\ 30'$ at RT. [a])*65K9*

4 Thermal expansion: Fig. 381.

5a Dielectric constant: Fig. 382.

Nr. 1B3-xv $Pb(Lu_{1/2}Ta_{1/2})O_3$

1a Dielectric anomaly in $Pb(Lu_{1/2}Ta_{1/2})O_3$ was found by Smolenskii and Agranovskaya in 1958. *58S3*

b

phase	II	I
state	(A)	P
crystal system	monoclinic	cubic
Θ	280	°C

$a = 4.153$ Å, $b = 4.107$ Å, $\beta = 90°\ 30'$ at RT. *65K9*

4 Lattice distortion: Fig. 383.
Thermal expansion: Fig. 384.

5 Dielectric constant: Fig. 385.

Nr. 1B3-xvi $Pb(Fe_{1/2}W_{1/2})O_3$

1a A synthesis of $Pb(Fe_{1/2}W_{1/2})O_3$ with perovskite structure was reported by Venevtsev et al. *64V3*

b The magnetic measurements confirmed the presence of the spinel phase in a sample of this composition. *65R5*

Nr. 1B3-xvii $Pb(Li_{1/4}Nb_{1/4}W_{1/2})O_3$ and sister crystals

1a Following composite perovskite compounds containing Pb were synthesized: *64V3* *65V3*

$Pb(Li_{1/4}Nb_{1/4}W_{1/2})O_3$	$Pb(Zn_{1/4}Mn_{1/4}Nb_{1/2})O_3$	$Pb(Co_{1/4}Mn_{1/4}W_{1/2})O_3$
$Pb(Mg_{1/4}Mn_{1/4}Nb_{1/2})O_3$	$Pb(Cd_{1/4}Mn_{1/4}Nb_{1/2})O_3$	$Pb(Ni_{1/4}Mn_{1/4}W_{1/2})O_3$
$Pb(Co_{1/4}Mn_{1/4}Nb_{1/2})O_3$	$Pb(Mg_{1/4}Mn_{1/4}Ta_{1/2})O_3$	$Pb(Cd_{1/4}Mn_{1/4}W_{1/2})O_3$
$Pb(Ni_{1/4}Mn_{1/4}Nb_{1/2})O_3$	$Pb(Mg_{1/4}Mn_{1/4}W_{1/2})O_3$	$Pb(Sc_{1/4}Cr_{1/4}Nb_{1/2})O_3$

Nr. 1B4-i $Pb(Mg_{1/3}Nb_{2/3})O_3$

1a Ferroelectricity in $Pb(Mg_{1/3}Nb_{2/3})O_3$ was discovered by Smolenskii and Agranovskaya in 1958. *58S3, 59S6*

b

phase	II	I
state	F	P
crystal system		cubic
space group		Pm3m-O_h^1
Θ	265[a])	°K

61B5, 60S7

[a])*67B9*

$\varrho = 8.12 \cdot 10^3$ kg m^{-3}, $a = 4.04$ Å at RT.
Transparent, pale yellow. *67B18*

2a	Crystal growth: Flux method (using PbO). Kyropoulos method.	59M5, 67B18
3	Crystal structure: Disordered perovskite.	61B5
4	Thermal expansion: Fig. 386.	
5a	Dielectric constant: Fig. 387, 388, 389.	
b	Nonlinear dielectric properties: $E = [(T - \Theta_p)(\varepsilon_0 C)^{-1}]\,P + \xi P^3 + \zeta P^5 + \cdots$, where $\Theta_p = 265$ °K, $C = (3.7 \pm 1.0) \cdot 10^5$ °K, and $\xi \cong 5.6 \cdot 10^8$ V m^5 C^{-3}.	67B9
c	Spontaneous polarization and coercive field: Fig. 390.	
7a	Piezoelectricity: Fig. 391.	
9a	Refractive index: $n = 2.56$ for 6328 Å at 299 °K. Birefringence: It was found that the crystals $Pb(Mg_{1/3}Nb_{2/3})O_3$ behave like optically isotropic crystals. An applied electric field causes double refraction. Fig. 392.	67B9
e	Quadratic electrooptic effect: $M_{11} - M_{12} = +0.015$ m^4 C^{-2}, $M_{44} = +0.008$ m^4 C^{-2} for 6328 Å at 299 °K.	67B9
14a	Domain structure: Clear domains were observed only in very thin wafers (e. g., $20 \cdot 10^{-6}$ m).	61B5

Nr. 1B4-ii $Pb(Zn_{1/3}Nb_{2/3})O_3$

1a	Ferroelectric $Pb(Zn_{1/3}Nb_{2/3})O_3$ crystal was synthesized by Bokov and Myl'nikova in 1960.	60B7
b	(see table below) $a = 4.04$ Å at RT. light yellow.	60B7
2a	Crystal growth: Flux method with PbO. The crystals were separated from the matrix solution by washing in acetic acid at RT for a long time.	60B7
5a	Dielectric constant: Fig. 393.	

phase	II	I
state	F	P
crystal system		cubic
Θ	140	°C

Nr. 1B4-iii $Pb(Cd_{1/3}Nb_{2/3})O_3$

1b	Dielectric anomaly in $Pb(Cd_{1/3}Nb_{2/3})O_3$ was reported by Venevtsev et al. in 1966.	65T5, 66V5

Nr. 1B4-iv $Pb(Co_{1/3}Nb_{2/3})O_3$

1a	Ferroelectricity in $Pb(Co_{1/3}Nb_{2/3})O_3$ was found by Bokov and Myl'nikova in 1960.	60B7
b	(see table below) $a = 4.04$ Å at RT. brown.	60B7
2a	Crystal growth: Flux method with PbO.	60B7
5a	Dielectric constant: Fig. 394.	

phase	II	I
state	F	P
crystal system		cubic
space group		Pm3m-O_h^1
Θ	−98	°C

Nr. 1B4-v $Pb(Ni_{1/3}Nb_{2/3})O_3$

1a Ferroelectricity in $Pb(Ni_{1/3}Nb_{2/3})O_3$ was discovered by SMOLENSKII and AGRANOVSKAYA in 1958. — *58S3, 59S6*

b

phase	II	I
state	F	P
crystal system		cubic
space group		$Pm3m\text{-}O_h^1$
Θ	153	°K

61B5, 60S7

$a = 4.03$ Å at RT. $\varrho = 8.55 \cdot 10^3$ kg m^{-3}.
yellowish green. — *59M5*

2a	Crystal growth: Flux method with PbO.	*59M5*
3	Crystal structure: Disordered perovskite.	*59M5*
4	Thermal expansion: Fig. 395.	*61B5*
5a	Dielectric constant: Fig. 396, 397, 398.	
9a	Birefringence: Fig. 399.	

Nr. 1B4-vi $Pb(Mg_{1/3}Ta_{2/3})O_3$

1a Ferroelectricity in $Pb(Mg_{1/3}Ta_{2/3})O_3$ was found by BOKOV and MYL'NIKOVA in 1960. — *60B7*

b

phase	II	I
state	F	P
crystal system		cubic
space group		$Pm3m\text{-}O_h^1$
Θ	−98	°C

60B7

$a = 4.02$ Å at RT.
light yellow.

2a	Crystal growth: Flux method with PbO.	*60B7*
3	Crystal structure: Disordered perovskite.	*60B7*
5a	Dielectric constant: Fig. 400.	

Nr. 1B4-vii $Pb(Co_{1/3}Ta_{2/3})O_3$

1a Ferroelectricity in $Pb(Co_{1/3}Ta_{2/3})O_3$ was found by BOKOV and MYL'NIKOVA in 1960. — *60B7*

b

phase	II	I
state	F	P
crystal system		cubic
space group		$Pm3m\text{-}O_h^1$
Θ	−140	°C

60B7

$a = 4.01$ Å at RT.
brown.

2a	Crystal growth: Flux method with PbO.	*60B7*
3	Crystal structure: Disordered perovskite.	*60B7*
5a	Dielectric constant: Fig. 401.	

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Nr. 1B4-viii $Pb(Ni_{1/3}Ta_{2/3})O_3$

1a	Ferroelectricity in $Pb(Ni_{1/3}Ta_{2/3})O_3$ was found by BOKOV and MYL'NIKOVA in 1960.	60B7
b	phase: II, I; state: F, P; crystal system: —, cubic; space group: —, Pm3m-O_h^1; Θ: −180 °C; $a = 4.01$ Å at RT. green.	60B7
2a	Crystal growth: Flux method.	60B7
3	Crystal structure: Disordered perovskite.	60B7
5a	Dielectric constant: Fig. 402.	

phase	II		I
state	F		P
crystal system			cubic
space group			Pm3m-O_h^1
Θ		−180	°C

Nr. 1B5-i $Pb(Mn_{2/3}W_{1/3})O_3$

1a	Dielectric and magnetic anomalies in $Pb(Mn_{2/3}W_{1/3})O_3$ were reported by ROGINSKAYA et al. in 1965.	65R5
b	(see table below) $a = c = 4.098$ Å, $b = 4.014$ Å, $\beta = 90°\ 23'$ at RT.	65R5
5a	Dielectric constant: Fig. 403.	
10	$\sigma = 2 \cdot 10^{11}\ \Omega^{-1}\ m^{-1}$.	65R5
11	Magnetic susceptibility: see Fig. 403. $\Theta_{p\,magn} = -75$ °K.	

phase	III		II		I
state	(A), (A_{magn})		(A), P_{magn}		P, P_{magn}
crystal system			monoclinic		cubic
Θ		203		473	°K

Nr. 1B5-ii $Pb(Fe_{2/3}W_{1/3})O_3$

1a	Ferroelectricity in $Pb(Fe_{2/3}W_{1/3})O_3$ was discovered by SMOLENSKII et al. in 1959.	59S7
b	(see table below) $a = 4.02$ Å at RT.	62B7, 65R5
2a	Flux method (PbO).	62B7
5a	Dielectric constant: Fig. 404.	
11	Magnetic susceptibility: see Fig. 404. Magnetization is a linear function of the magnetic field intensity up to 8000 Oe. Effective magnetic moment: 4.2 μ_B.	62B7
12b	ESR: Fig. 405.	

phase	III		II		I
state	F, A_{magn}		P, A_{magn}		P, P_{magn}
crystal system			cubic		cubic
Θ		178		363	°K

1C Solid solutions with perovskite-type oxides as end members

Nr. 1C-a1 $NaNbO_3$-$KNbO_3$

1b	Phase diagram: Fig. 406, 407, 408. Lattice parameters: Fig. 409.	
5a	Dielectric constant: Fig. 410; see Tab. 60. Polarization and coercive field: Fig. 411.	
6a	Transition energy: Tab. 59.	
7a	Electromechanical properties: Fig. 412 ··· 417; Tab. 60.	

Tab. 59. $(Na_{1-x}K_x)NbO_3$. Transition energy ΔQ_m. [54S3]

x	Lower phase change	Upper phase change
1.00 ($KNbO_3$)	85 cal/mole	190 cal/mole
0.10	20 cal/mole	60 cal/mole
0 ($NaNbO_3$)	—	50 cal/mole

Tab. 60. $(Na_{0.5}K_{0.5})NbO_3$ (ceramics). Electric and electromechanical constants. [59E1]

Dielectric constant (100 kHz)	290
Dissipation factor (100 kHz)	≈4.0%
Specific resistivity ϱ	$10^{10}\ \Omega$ m
Density ϱ	$4.25 \cdot 10^3$ kg m^{-3}
Poisson's ratio (assumed)	0.27
Coupling factor k_p	0.34 ⋯ 0.39
Frequency constant $f_R r$	1.67 kHz m
Mechanical Q_{mech} (radial)	130
Young's modulus E	$1.04 \cdot 10^{11}$ N m^{-2}
Piezoelectric constant $-d_{31}$	$32 \cdot 10^{-12}$ C N^{-1}
Piezoelectric constant $-g_{31}$	$12.6 \cdot 10^{-3}$ m^2 C^{-1}
Piezoelectric constant d_{33}^*	$80 \cdot 10^{-12}$ C N^{-1}
Piezoelectric constant g_{33}^*	$31.5 \cdot 10^{-3}$ m^2 C^{-1}
Coupling factor k_{33}^*	0.51

Nr. 1C-a2 $NaNbO_3$-$NaTaO_3$

1b	Phase diagram: Fig. 418. Lattice parameters: Fig. 419.
4	Thermal expansion: Fig. 420.
5a	Dielectric constant: Fig. 421.
9a	Birefringence: Fig. 422.

Nr. 1C-a3 $NaNbO_3$-$NaSbO_3$

1a	Curie temperature: Fig. 423.

Nr. 1C-a4 $KNbO_3$-$KTaO_3$

1	Phase diagram: Fig. 424, 425.
5a	Dielectric properties: Fig. 426, 427. Θ_f: see Tab. 61.
6	Thermal properties: Fig. 428; Tab. 61.
9	See 1C-a5 for optical properties of $K(Ta_{0.35}Nb_{0.65})O_3$ (KTN).

Tab. 61. $K(Nb_{1-x}Ta_x)O_3$. L: latent heat, Θ_f: Curie point, A: constant in the formula for free energy $= A(T-\Theta_p)P^2 + \cdots$, P_{calc}: P_s calculated for $T = \Theta_f$. [59H1]

x	L cal mol^{-1}	Θ_f °K	A 10^5 °K^{-1}	P_{calc} 10^{-2} C m^{-2}
0	110 ± 10	679	2.6	27
0.06	46 ± 4	656	2.7	17.7
0.12	10 ± 2	623	2.85	7.9
0.18	4.0 ± 2	591	3.05	5.1

Nr. 1C-a5 $K(Ta_{0.35}Nb_{0.65})O_3$ (KTN)

For general properties of $KNbO_3$-$KTaO_3$ see 1C-a4.

9b	Electroreflectance: Fig. 429.
d	Faraday rotation: Fig. 430. See also Tab. 44.

Nr. 1C-a6 $CaTiO_3$-$SrTiO_3$

1b	Phase diagram: Fig. 431, 432, 433. Lattice parameters: Fig. 434.
5a	Dielectric constant: Fig. 435, 436.
c	Spontaneous polarization: Fig. 437.

Nr. 1C-a7 $CaTiO_3$-$BaTiO_3$

1b	Phase diagram: Fig. 438, 439, 440. Lattice parameters: Fig. 441.
5a	Dielectric constant: Fig. 442, 443.
6b	Thermal conductivity: Fig. 444.
7a	Electromechanical property: Tab. 62. See Fig. 183 and Tab. 40.

* Estimated values.

Tab. 62. $(Ba_{1-x}Ca_x)TiO_3$ (ceramics, pure $BaTiO_3$ base). d_{31} and d_{33} at RT. [57B4]

x	ϱ 10^3 kg m^{-3}	ϱ_X 10^3 kg m^{-3}	d_{31} 10^{-12}CN^{-1}	d_{33} 10^{-12}CN^{-1}	$-d_{33}/d_{31}$	Porosity $(1-(\varrho/\varrho_X))$
0	5.85	6.017	−97.5	229	2.35	0.028
0.05	5.70	5.85	−66.6	167	2.51	0.026
0.07	5.68	5.80	−58.0	150	2.58	0.021
0.09	5.65	5.74	−52.1	139	2.67	0.016
0.12	5.55	5.66	−43.4	124.5	2.88	0.019

Nr. 1C-a8 $CaTiO_3$-$PbTiO_3$

1b	Curie temperature: Fig. 445. Lattice parameter: Fig. 446.

Nr. 1C-a9 $SrTiO_3$-$BaTiO_3$

1b	Phase diagram: Fig. 447 ··· 450. Lattice parameter: Fig. 451; see Fig. 448.
5a	Dielectric constant: Fig. 452. Microwave dielectric loss: Tab. 63.
6a	Specific heat: Fig. 453.
10b	Conductivity associated with doping: Fig. 454, 455, 456.

Tab. 63. $(Ba_{1-x}Sr_x)TiO_3$. Dielectric loss: α, β, γ at 20 GHz. [62R4]. $(T-\Theta_p)\tan\delta = \alpha + \beta T + \gamma T^2$.

Sample		Heat treatment	Grain size μ	Θ_p °K	α °K	$\beta \cdot 10^4$	$\gamma \cdot 10^6$ (°K)$^{-1}$
Polycristalline	$SrTiO_3$	Hot pressed and fired in air at 900 °C for 10 h	1	37	0.33	7.7	4.3
		Refired at 1200 °C in air for 10 h	3	37	0.26	5.5	4.7
		Refired at 1400 °C in air for 10 h	15	37	0.17	4.4	4.2
		Refired at 1500 °C in O_2 for 6 h	30	37	0.08	4.5	3.7
	$Ba_{0.2}Sr_{0.8}TiO_3$	Hot pressed and fired in O_2 at 1500 °C for 10 h	30	105	0.6	9	2.5
	$Ba_{0.5}Sr_{0.5}TiO_3$	Hot pressed and fired in O_2 at 1500 °C for 10 h	30	218	2.0	(9)[a]	(2.5)
	$Ba_{0.7}Sr_{0.3}TiO_3$	Ceramic fired to 1375 °C in air for 1 h	8	280	2.2	(9)	(2.5)
	$Ba_{0.8}Sr_{0.2}TiO_3$	Ceramic fired to 1300 °C in air for 1 h	8	324	1.6	(9)	(2.5)
Single crystal	$SrTiO_3$	None	∞	37	0	6.53	2.54
	$SrTiO_3$+0.1% Gd^{3+}	None	∞	37	0.033	(6.53)	(2.54)
	$SrTiO_3$+0.03% Fe^{3+}	None	∞	37	0.043	(6.53)	(2.54)

Nr. 1C-a10 $SrTiO_3$-$PbTiO_3$

1b	Curie temperature: Fig. 457. Lattice parameter: Fig. 458.
5a	Dielectric constant: Fig. 459. Curie constant: Fig. 460.
6a	Transition heat: Fig. 461.

Nr. 1C-a11 $BaTiO_3$-$PbTiO_3$

1b	Phase diagram: Fig. 462. Lattice parameter: Fig. 463.
5a	Dielectric constant: Fig. 464.
6a	Specific heat: Fig. 465. Transition heat: Fig. 466.
7	Electromechanical properties: see 1A-8.
16	Radiation damage: Fig. 467.

[a]) Values in parentheses indicate that these values were assumed in order to determine α.

Nr. 1C-a12 $CaZrO_3$-$BaZrO_3$	1b	Lattice parameter: Fig. 468.
Nr. 1C-a13 $CaZrO_3$-$PbZrO_3$	1b	Phase diagram: Fig. 469.
	4	Thermal expansion: Fig. 470.
	5a	Dielectric constant: Fig. 471.
Nr. 1C-a14 $SrZrO_3$-$PbZrO_3$	1b	Phase diagram: Fig. 472, 473. Lattice parameter: Fig. 474.
	4	Thermal expansion: Fig. 475, 476, 477; Tab. 64.
	5a	Dielectric constant: Fig. 478, 479.
	c	Polarization: Fig. 480.
	6a	Specific heat: Fig. 481. Transition heat: Tab. 65.

Tab. 64. $PbZrO_3$, $(Pb_{0.95}Sr_{0.05})ZrO_3$, and $(Pb_{0.925}Ba_{0.075})ZrO_3$. $\Delta V/V$. ΔV: anomalous volume change at the transition point. [54S2]

Composition	$\Delta V/V$ [10^{-4}] Lowest phase	Intermediate phase
$PbZrO_3$	−41 at 230 °C	–
$(Pb_{0.925}Ba_{0.075})ZrO_3$	−43 at 150 °C	+24 at 190 °C
$(Pb_{0.95}Sr_{0.05})ZrO_3$	−30 at 210 °C	−20 at 230 °C

Tab. 65. $PbZrO_3$, $(Pb_{0.95}Sr_{0.05})ZrO_3$, and $(Pb_{0.925}Ba_{0.075})ZrO_3$. ΔQ_m. [52S2]

Composition	ΔQ_m [cal mol^{-1}] Lower transition	Upper transition
$PbZrO_3$	–	440
$(Pb_{0.925}Ba_{0.075})ZrO_3$	190	230
$(Pb_{0.95}Sr_{0.05})ZrO_3$	180	230

Nr. 1C-a15 $BaZrO_3$-$PbZrO_3$	1b	Phase diagram: Fig. 482. Lattice parameter: Fig. 483.
	4	Thermal expansion: Fig. 484.
	5a	Dielectric constant: Fig. 485 ··· 488.
	c	Coercive field: Fig. 489.
	8	Elastic properties: Fig. 490.
Nr. 1C-a16 $CaHfO_3$-$PbHfO_3$	1b	Phase diagram: Fig. 491.
	5a	Dielectric constant: Fig. 492.
Nr. 1C-a17 $SrHfO_3$-$PbHfO_3$	1b	Phase diagram: Fig. 493.
	5a	Dielectric constant: Fig. 494.
Nr. 1C-a18 $BaHfO_3$-$PbHfO_3$	1b	Phase diagram: Fig. 495.
Nr. 1C-a19 $CaSnO_3$-$SrSnO_3$	1b	Lattice parameter: Fig. 496.
Nr. 1C-a20 $BaSnO_3$-$SrSnO_3$	1b	Lattice parameter: see Fig. 496.
Nr. 1C-a21 $BaSnO_3$-$PbO:SnO_2$	1b	Phase diagram: Fig. 497.
	5a	Dielectric constant: Fig. 498.
Nr. 1C-a22 $CaTiO_3$-$CaZrO_3$	1b	Lattice parameter: Fig. 499.

Nr. 1C-a23 $BaTiO_3$-$BaZrO_3$

1b	Phase diagram: Fig. 500. Lattice parameter: Fig. 501.	
2a	Phase diagram: Fig. 502.	
5a	Dielectric constant: Fig. 503.	
8a	Elastic property: Fig. 504	

Nr. 1C-a24 $BaTiO_3$-$BaHfO_3$

1b	Phase diagram: Fig. 505. Lattice parameter: Fig. 506.	
5a	Dielectric constant: Fig. 507.	

Nr. 1C-a25 $BaTiO_3$-$BaSnO_3$

1b	Phase diagram: Fig. 508. See also	*59I2*
2a	Phase diagram: Fig. 509.	
4	Thermal expansion: Fig. 510.	
5a	Dielectric constant: Fig. 511.	

Nr. 1C-a26 $BaTiO_3$-$BaUO_3$

1b	Lattice parameter: Fig. 512.	

Nr. 1C-a27 $PbTiO_3$-$PbZrO_3$

$Pb(Zr_xTi_{1-x})O_3$ with $x = 0.5 \cdots 0.6$; for electromechanical properties of these very important piezoelectric materials, see 1C-a28.

1a	Ferro- and antiferroelectric phase transitions in the $PbTiO_3$-$PbZrO_3$ system were revealed in 1952 by Shirane, Suzuki and Takeda.	*52S6, 52S4, 52S3*
b	Phase diagram at high temperature: Fig. 513. Phase diagram: Fig. 514, 515. Lattice parameter: Fig. 516, 517.	
2	Flux method:	*62I1, 64F6, 67F7*
4	Lattice distortion: Fig. 518a, b, 519. Thermal expansion: Fig. 520, 521, 522.	
5a	Dielectric constant: Fig. 523 ⋯ 526.	
c	Spontaneous polarization: Fig. 527. Critical field: Fig. 528.	
6	Specific heat: Fig. 529, 530. Transition energy: Tab. 66.	
7, 8	Electromechanical properties: see 1C-a28.	
9	Birefringence: Fig. 531a, b, c.	
16	Radiation damage: Fig. 532.	

Tab. 66. Pb(Zr-Ti)O_3. Transition energy and entropy. [*53S1*]. x: atomic per-cent of $PbTiO_3$; $d\Theta/dx$: shift of the transition temperature with x; $dS(d\Theta/dx)$: it may be assumed that the free energy should decrease with the rate of $dS(d\Theta/dx)$ with increasing x.

Kind of the phase change	Θ °C	ΔQ_m cal mol^{-1}	ΔS_m cal mol^{-1} °K^{-1}	$d\Theta/dx$	$dS(d\Theta/dx)$
$A_\alpha \to P_\alpha$	$230 > T > 225$	400	0.8	—	(−5.8)
$A_\alpha \to A_\beta$	225	110	0.22	−16	−3.5
$A_\beta \to P_\alpha$	230	290	0.58	− 4	−2.3
$A_\alpha \to F_\alpha$	240	—	—	−19	—
$F_\alpha \to P_\alpha$	217	250	0.51	+ 1.0	+0.5
$A_\beta \to F_\alpha$	—	40	0.08	—	—

Nr. 1C-a28 $Pb(Zr_xTi_{1-x})O_3$ ($x = 0.5 \cdots 0.6$, lead zirconate-titanate)
For general properties of $PbTiO_3$-$PbZrO_3$ see 1C-a27.

1a	JAFFE, ROTH, and MARZULLO discovered the excellent piezoelectric performances of $Pb(Zr\text{-}Ti)O_3$ ceramics in 1954. PZT is the trade mark of this substance developed by Clevite Corporation, Cleveland, Ohio, USA.	*54J1*
5a	Dielectric constants: Fig. 533 and Fig. 539, 540, 541, 543, 544.	
7, 8	Electromechanical properties (ceramics): Tab. 67; Fig. 534 ··· 538; Tab. 68 ··· 72; Fig. 539 ··· 542; Tab. 73; Fig. 543 ··· 554.	
10	Electrical conductivity: see For breakdown, see	*63G1, 61S14* *59G2*

Tab. 67. $Pb(Ti_{1-x}Zr_x)O_3$ [$x = 0.48 \cdots 0.60$] (ceramics). Electromechanical constants at RT. [*60B3*]

Zr/Ti atom ratio	k_{31}	k_p	k_{15}	k_{33}	$\varkappa_{11}^T$	$\varkappa_{11}^S$	$\varkappa_{33}^T$	$\varkappa_{33}^S$ obs	$\varkappa_{33}^S$ calc
48/52	0.170	0.289	0.408	0.435	663	551	666	540	537
50/50	0.230	0.397	0.504	0.546	855	631	846	585	585
52/48	0.313	0.529	0.694	0.670	1180	612	730	399	389
54/46	0.280	0.470	0.701	0.626	990	504	450	253	268
56/44	0.267	0.450	0.657	0.619	840	477	423	246	258
58/42	0.254	0.428	0.646	0.607	751	437	397	243	246
60/40	0.238	0.400	0.625	0.585	672	410	376	240	245

	s_{11}^E	s_{11}^D	s_{33}^E	s_{33}^D	s_{44}^E	s_{44}^D	s_{66}	s_{12}^E	s_{12}^D	s_{13}^E	s_{13}^D	Density ϱ
	10^{-12} m² N⁻¹											10^3 kgm⁻³
48/52	10.8	10.5	10.9	8.83	28.3	23.6	28.3	−3.35	−3.66	−3.21	−2.40	7.59
50/50	12.4	11.7	13.3	9.35	32.8	24.5	32.9	−4.06	−4.72	−4.22	−2.60	7.55
52/48	13.8	12.4	17.1	9.35	48.2	25.0	38.4	−4.07	−5.38	−5.80	−2.56	7.55
54/46	11.6	10.7	14.8	9.0	45.0	22.9	29.9	−3.33	−4.24	−4.97	−2.68	7.62
56/44	11.0	10.2	14.0	8.65	39.8	22.6	28.4	−3.22	−4.01	−4.63	−2.57	7.59
58/42	10.5	9.85	12.8	8.10	37.7	21.9	27.1	−3.07	−3.75	−4.12	−2.33	7.64
60/40	10.4	9.75	12.05	7.92	36.9	22.5	26.7	−2.96	−3.55	−3.72	−2.17	7.60

	g_{31}	g_{33}	g_{15}	$g_{33}-g_{31}$	d_{31}	d_{33}	d_{15}	$d_{33}-d_{31}$	$s_{33}^D+s_{11}^D-2s_{13}^D$
	10^{-3} m² C⁻¹				10^{-12} C N⁻¹				10^{-12} m² N⁻¹
48/52	− 7.3	18.7	28.4	26.0	43.0	110	166	153	24.1
50/50	− 9.35	23.1	33.2	32.4	70.0	173	251	243	26.2
52/48	−14.5	34.5	47.2	49.0	93.5	223	494	316	26.9
54/46	−15.1	38.1	50.3	53.2	60.2	152	440	212	25.1
56/44	−14.5	37.8	48.0	52.3	54.3	142	357	196	24.0
58/42	−13.9	36.7	48.8	50.6	48.9	129	325	178	22.6
60/40	−13.3	35.2	49.3	48.5	44.2	117	293	161	22.0

	Q_{mech}	Q_E (=1/tan δ)	P	c_{33}^D	$\frac{-s_{12}^E}{s_{11}^E}$	$\frac{-s_{12}^D}{s_{11}^D}$	$\frac{-s_{13}^E}{\sqrt{s_{33}^E s_{11}^E}}$	$\frac{-s_{13}^D}{\sqrt{s_{33}^D s_{11}^D}}$
			10^{-2} C m⁻²	10^{10} N m⁻²				
48/52	1170	380	17	14.0	0.310	0.349	0.296	0.250
50/50	950	370	27	13.5	0.328	0.404	0.329	0.249
52/48	860	360	36	13.4	0.295	0.434	0.376	0.238
54/46	680	300	42.5	14.8	0.288	0.396	0.380	0.273
56/44	490	190	48	15.3	0.293	0.394	0.373	0.274
58/42	500	200	43	15.8	0.292	0.381	0.355	0.261
60/40	600	210	33	15.6	0.285	0.365	0.332	0.247

Tab. 68. $(Pb_{1-x}Sr_x)(Zr_{1-y}Ti_y)O_3$ and $(Pb_{1-x}Ca_x)(Zr_{1-y}Ti_y)O_3$ (modified ceramics). Effects of Ca and Sr on electromechanical properties. [*59K4*]

Intended composition	ϱ_a 10^3 kgm^{-3}	$\varkappa$ at 1 kHz	24 hours after poling: $\varkappa$ at 1 kHz	tan δ % at 1 kHz	k_p	d_{31} 10^{-12} CN^{-1}	g_{31} 10^{-3} m^2C^{-1}	$(s_{11}^E)^{-1}$ 10^{10} Nm^{-2}	Θ_f °C
$Pb(Zr_{0.53}Ti_{0.47})O_3$	7.40	736	544	0.5	0.48	71	14.7	7.67	385
$Pb(Zr_{0.53}Ti_{0.47})O_3$	7.39	707	542	0.4	0.47	69	14.4	7.76	
$Pb_{0.99}Ca_{0.01}(Zr_{0.53}Ti_{0.47})O_3$	7.42	729	624	0.5	0.49	77	13.9	7.89	
$Pb_{0.99}Sr_{0.01}(Zr_{0.53}Ti_{0.47})O_3$	7.42	755	584	0.6	0.49	75	14.5	7.68	
$Pb_{0.95}Ca_{0.05}(Zr_{0.53}Ti_{0.47})O_3$	7.26	832	973	0.5	0.44	88	10.2	7.62	
$Pb_{0.95}Sr_{0.05}(Zr_{0.53}Ti_{0.47})O_3$	7.47	920	1002	0.4	0.50	101	11.4	7.65	360
$Pb_{0.92}Ca_{0.08}(Zr_{0.53}Ti_{0.47})O_3$	6.86	794	888	0.4	0.32	60	7.6	7.85	
$Pb_{0.925}Sr_{0.075}(Zr_{0.53}Ti_{0.47})O_3$	7.29	942	1094	0.3	0.50	103	10.6	7.94	
$Pb_{0.90}Sr_{0.10}(Zr_{0.53}Ti_{0.47})O_3$	7.22	997	1129	0.3	0.49	103	10.3	7.95	290
$Pb_{0.875}Sr_{0.125}(Zr_{0.47}Ti_{0.53})O_3$	7.09	609	663	0.3	0.28	40	6.8	9.91	
$Pb_{0.875}Sr_{0.125}(Zr_{0.50}Ti_{0.50})O_3$	7.11	813	880	0.3	0.33	57	7.3	9.05	
$Pb_{0.875}Sr_{0.125}(Zr_{0.52}Ti_{0.48})O_3$	7.10	973	1149	0.3	0.44	91	9.0	8.32	
$Pb_{0.875}Sr_{0.125}(Zr_{0.53}Ti_{0.47})O_3$	7.14	1076	1237	0.4	0.47	100	9.1	8.06	265
$Pb_{0.875}Sr_{0.125}(Zr_{0.54}Ti_{0.46})O_3$	7.16	1095	1325	0.6	0.51	119	10.1	7.51	
$Pb_{0.875}Sr_{0.125}(Zr_{0.56}Ti_{0.44})O_3$	7.14	1105	1210	0.4	0.51	116	10.8	7.31	
$Pb_{0.875}Sr_{0.125}(Zr_{0.59}Ti_{0.41})O_3$	7.17	919	585	0.4	0.45	66	12.7	8.39	
$Pb_{0.85}Sr_{0.15}(Zr_{0.53}Ti_{0.47})O_3$	6.90	1106	1260	0.5	0.43	97	8.7	7.68	242
$Pb_{0.80}Sr_{0.20}(Zr_{0.50}Ti_{0.50})O_3$	6.56	941	970	0.6	0.29	56	6.5	8.11	
$Pb_{0.80}Sr_{0.20}(Zr_{0.53}Ti_{0.47})O_3$	6.48	1212	1257	0.5	0.34	86	7.8	7.05	
$Pb_{0.80}Sr_{0.20}(Zr_{0.54}Ti_{0.46})O_3$	6.36	1182	1341	0.8	0.35	91	7.7	6.18	
$Pb_{0.80}Sr_{0.20}(Zr_{0.55}Ti_{0.45})O_3$	6.36	1200	1337	0.8	0.34	86	7.3	6.42	
$Pb_{0.80}Sr_{0.20}(Zr_{0.56}Ti_{0.44})O_3$	6.35	1107	1113	0.7	0.35	81	8.2	6.50	

Tab. 69. $Pb(Zr\text{-}Ti)O_3$ (ceramics, modified). Electromechanical properties of $Pb(Zr_{0.54}Ti_{0.46})O_3$ with five-valent additives. [*59K5*]. $f_R \cdot r$: radial frequency constant

Addition wt. %	ϱ_a 10^3 kgm^{-3}	Before poling: $\varkappa$ at 1 kHz	Before poling: tan δ % at 1 kHz	24 hours after poling: $\varkappa$ at 1 kHz	tan δ % at 1 kHz	k_p	$f_R \cdot r$ Hz·m	d_{31} 10^{-12} CN^{-1}	Q_{mech}	Θ_f °C
None	7.41	707	0.3	537	0.4	0.49	1641	71		390
None	7.29	706	0.4	513	0.5	0.50	1687	69		387
0.1 Nb_2O_5	7.26	598	0.3	508	0.4	0.38	1643	54		
0.5 Nb_2O_5	6.96	732	2.1	790	2.0	0.46	1443	94		
0.8 Nb_2O_5	7.36	965	1.6	1166	1.5	0.48	1606	105		
1.0 Nb_2O_5	7.36	1064	1.8	1308	1.6	0.53	1563	126	61	
1.0 Nb_2O_5	7.60	1055	2.2	1242	2.2	0.54	1538	125		361
1.2 Nb_2O_5	7.34	1011	2.0	1167	1.7	0.48	1614	104	70	
1.4 Nb_2O_5	7.37	1057	2.2	1218	1.9	0.50	1584	113	69	
1.7 Nb_2O_5	7.39	1058	2.0	1218	1.8	0.47	1594	105		
2.0 Nb_2O_5	7.37	1074	2.1	1202	2.0	0.50	1550	115		344
0.5 Nb_2O_5 } 0.5 La_2O_3 }	7.39	1169	2.1	1377	2.0	0.57	1491	146	48	369
1.0 Ta_2O_5	7.31	989	1.5	1187	1.5	0.49	1563	111	61	
1.0 Ta_2O_5	7.22	918	2.0	1121	2.1	0.50	1525	114		368
2.0 Ta_2O_5	7.49	1062	2.2	1230	2.1	0.50	1547	115		
2.0 Ta_2O_5	7.40	1077	1.8	1275	1.8	0.48	1581	111		364
2.5 Ta_2O_5	7.23	959	2.7	1112	2.4	0.36	1518	82	28	
5.0 Ta_2O_5	6.75	995	2.5	1052	2.6	0.33	1508	76		

Tab. 70. $Pb(Zr\text{-}Ti)O_3$ (ceramics, modified). Electromechanical properties of $Pb(Zr_{0.54}Ti_{0.46})O_3$ with three-valent additives. [59K5]. $f_R \cdot r$: radial frequency constant

Addition wt. %	ϱ_a 10^3 kg m^{-3}	Before poling		24 hours after poling					Θ_f °C
		$\varkappa$ at 1 kHz	tan δ % at 1 kHz	$\varkappa$ at 1 kHz	tan δ % at 1 kHz	k_p	$f_R \cdot r$ Hz·m	d_{31} 10^{-12} CN^{-1}	
None	7.41	707	0.3	537	0.4	0.49	1641	71	390
None	7.29	706	0.4	513	0.5	0.50	1687	69	387
1.0 Y_2O_3	7.26	796	0.9	841	1.0	0.34	1547	66	374
1.0 La_2O_3	7.46	1187	1.9	1483	2.0	0.53	1510	138	
1.0 La_2O_3	7.47	1139	2.2	1387	2.1	0.52	1522	130	339
1.0 Nd_2O_3	7.43	1111	1.6	1395	1.8	0.49	1512	123	
1.0 Nd_2O_3	7.37	1101	1.9	1354	1.8	0.48	1511	119	348
1.0 didymia	7.41	1122	2.2	1341	2.2	0.50	1499	125	
2.0 La_2O_3	7.49	1296	2.6	1545	2.3	0.51	1545	132	
1.0 La_2O_3	7.20	1375	2.1	1792	1.7	0.51	1528	147	
1.0 Nd_2O_3	7.35	1362	2.2	1776	1.9	0.49	1558	136	
0.1 La_2O_3	6.75	790	0.4	870	0.6	0.42	1505	88	
0.2 La_2O_3	6.45	686	0.7	735	0.9	0.37	1419	78	
0.4 La_2O_3	6.44	942	1.4	1100	1.5	0.42	1407	109	
0.8 La_2O_3	7.19	1288	1.8	1682	1.8	0.49	1516	139	
1.0 La_2O_3	7.50	1255	2.4	1532	2.4	0.50	1550	128	

Tab. 71. Electromechanical properties of $Pb(Zr_{1-x}Ti_x)O_3$ (ceramics), modified with additives of 1 wt% Nb. [59K5]. $f_R \cdot r$: radial frequency constant

Base composition	ϱ_a 10^3 kg m^{-3}	Before poling		24 hours after poling					
		$\varkappa$ at 1 kHz	tan δ % at 1 kHz	$\varkappa$ at 1 kHz	tan δ % at 1 kHz	k_p	$f_R \cdot r$ Hz·m	d_{31} 10^{-12} CN^{-1}	Q_{mech}
$Pb(Zr_{0.50}Ti_{0.50})O_3$	7.38	879	1.5	1041	1.2	0.42	1696	82	81
$Pb(Zr_{0.51}Ti_{0.49})O_3$	7.31	975	1.6	1188	1.3	0.45	1642	97	73
$Pb(Zr_{0.52}Ti_{0.48})O_3$	7.39	985	1.5	1200	1.4	0.45	1640	97	76
$Pb(Zr_{0.53}Ti_{0.47})O_3$	7.43	1092	1.8	1371	1.4	0.53	1547	130	61
$Pb(Zr_{0.54}Ti_{0.46})O_3$	7.44	1051	1.8	1296	1.7	0.54	1549	128	62
$Pb(Zr_{0.55}Ti_{0.45})O_3$	7.40	955	2.4	973	2.0	0.56	1524	117	55
$Pb(Zr_{0.56}Ti_{0.44})O_3$	7.38	818	2.8	745	2.5	0.53	1601	93	56
$Pb(Zr_{0.57}Ti_{0.43})O_3$	7.41	750	3.0	684	2.5	0.50	1636	82	60
$Pb(Zr_{0.58}Ti_{0.42})O_3$	7.41	713	3.0	630	2.8	0.49	1676	75	62

Tab. 72. Electromechanical properties of $(Pb_{0.95}Sr_{0.05})(Zr_{0.54}Ti_{0.46})O_3$ (ceramics) with Nb_2O_5 or Ta_2O_5. [59K5]. $f_R \cdot r$: radial frequency constant

Addition wt. %	ϱ_a 10^3 kg m^{-3}	Before poling		24 hours after poling					Θ_f °C
		$\varkappa$ at 1 kHz	tan δ % at 1 kHz	$\varkappa$ at 1 kHz	tan δ % at 1 kHz	k_p	$f_R \cdot r$ Hz·m	d_{31} 10^{-12} CN^{-1}	
1.0 Nb_2O_5	7.34	1291	2.0	1609	2.0	0.56	1512	153	306
2.0 Nb_2O_5	7.22	1380	2.4	1662	2.1	0.47	1562	127	
3.0 Nb_2O_5	6.63	1125	2.1	1301	2.1	0.36	1550	91	
2.0 Ta_2O_5	7.33	1343	2.3	1695	2.0	0.54	1517	151	296

Tab. 73. PZT (commercial modified ceramics). Electromechanical constants at RT. [66b1]

Substance	$\varkappa_{11}^T$	$\varkappa_{11}^S$	$\varkappa_{33}^T$	$\varkappa_{33}^S$	d_{15}	d_{31}	d_{33}	e_{15}	e_{31}	e_{33}	g_{15}	g_{31}	g_{33}	h_{15}
					10^{-12} C N^{-1}			C m^{-2}			10^{-3} m^2 C^{-1}			10^8 N C^{-1}
PZT-2	990	504	450	260	440	−60.2	152	9.8	−1.86	9.0	50.3	−15.1	38.1	21.9
PZT-4	1475	730	1300	635	496	−123	289	12.7	−5.2	15.1	39.4	−11.1	26.1	19.7
PZT-5A	1730	916	1700	830	584	−171	374	12.3	−5.4	15.8	38.2	−11.4	24.8	15.2
PZT-5H	3130	1700	3400	1470	741	−274	593	17.0	−6.55	23.3	26.8	−9.11	19.7	11.3
PZT-6A			1100			−77	195					−7.9	17.0	
PZT-6B	515	441	500	420	135	−29	76	4.8	−0.96	7.4	29.6	−6.6	17.3	12.2
PZT-7A	840	450	425	235	368	−61	153	9.3	−2.15	9.7	49.5	−16.2	40.7	23.4
PZT-8			1000			−95	215					−10.5	24.5	

Substance	h_{31}	h_{33}	k_{15}	k_{31}	k_{33}	k_p	s_{11}^E	s_{11}^D	s_{33}^E	s_{33}^D	s_{12}^E	s_{12}^D	s_{13}^E	s_{13}^D
	10^8 N C^{-1}						10^{-12} m^2 N^{-1}							
PZT-2	−8.1	39.2	0.701	0.28	0.626	0.47	11.6	10.7	14.8	9.0	−3.33	−4.24	−4.97	−2.68
PZT-4	−9.2	26.8	0.71	0.334	0.70	0.58	12.3	10.9	15.5	7.90	−4.05	−5.42	−5.31	−2.10
PZT-5A	−7.3	21.5	0.685	0.344	0.705	0.60	16.4	14.4	18.8	9.46	−5.74	−7.71	−7.22	−2.98
PZT-5H	−5.05	18.0	0.675	0.388	0.752	0.65	16.5	14.05	20.7	8.99	−4.78	−7.27	−8.45	−3.05
PZT-6A				0.229	0.54	0.39	11.5	10.9			−3.45	−4.05		
PZT-6B	−2.6	19.9	0.377	0.145	0.375	0.25	9.0	8.8	9.35	8.05	−3.0	−3.2	−3.1	−2.6
PZT-7A	−10.4	46.6	0.68	0.306	0.67	0.52	10.7	9.7	13.9	7.65	−3.2	−4.2	−4.6	−2.3
PZT-8				0.295	0.60	0.50	11.1	10.1	13.9	8.9				

Substance	s_{44}^E	s_{44}^D	s_{66}	c_{11}^E	c_{11}^D	c_{33}^E	c_{33}^D	c_{12}^E	c_{12}^D	c_{13}^E	c_{13}^D	c_{44}^E	c_{44}^D	c_{66}
	10^{-12} m^2 N^{-1}			10^9 N m^{-2}										
PZT-2	45.0	22.9	29.9	135	136	113	148	67.9	69.3	68.1	61.2	22.2	43.7	33.4
PZT-4	39.0	19.3	32.7	139	145	115	159	77.8	83.9	74.3	60.9	25.6	51.8	30.6
PZT-5A	47.5	25.2	44.3	121	126	111	147	75.4	80.9	75.2	65.2	21.1	39.7	22.6
PZT-5H	43.5	23.7	42.6	126	130	117	157	79.5	82.8	84.1	72.2	23.0	42.2	23.5
PZT-6A			29.9											
PZT-6B	28.2	24.2	24.0	168	169	163	177	85.1	86.2	84.0	82.4	35.4	41.3	41.7
PZT-7A	39.5	21.2	27.8	148	157	131	175	76.2	85.4	74.2	73.0	25.3	47.2	36.0
PZT-8			29.6											

Nr. 1C-a29 $PbTiO_3$-$PbHfO_3$	1b	Phase diagram: Fig. 555, 556
Nr. 1C-a30 $PbTiO_3$-$PbO:SnO_2$	1b	Phase diagram: Fig. 557.
	5a	Dielectric constant: Fig. 558.
Nr. 1C-a31 $PbZrO_3$-$PbHfO_3$	1b	Phase diagram: Fig. 559.
Nr. 1C-a32 $PbZrO_3$-$PbO:SnO_2$	1b	Phase diagram: Fig. 560. Lattice parameter: Fig. 561.
	4	Thermal expansion: Fig. 562, 563.
	5a	Dielectric constant: Fig. 564a, b.
Nr. 1C-a33 $LaFeO_3$-$BiFeO_3$	1b	Phase diagram: Fig. 565. Lattice parameter: Fig. 566a, b.
	5a	Dielectric constant: Fig. 567.
	11	Magnetization: see Fig. 565.
Nr. 1C-b1 $NaNbO_3$-$KTaO_3$	1b	Phase diagram: Fig. 568. Lattice parameter: Fig. 569.
	4	Thermal expansion: Fig. 570.
	5a	Dielectric constant: Fig. 571.
Nr. 1C-b2 $NaNbO_3$-$KSbO_3$	1a	Curie temperature: see Fig. 423.
Nr. 1C-b3 $BaTiO_3$-$PbZrO_3$	4	Thermal expansion: Fig. 572.
	5a	Dielectric constant: Fig. 573.
Nr. 1C-b4 $BaTiO_3$-$PbO:SnO_2$	1b	Phase diagram: Fig. 574.
	5a	Dielectric constant: Fig. 575.
Nr. 1C-b5 $PbTiO_3$-$CaZrO_3$	1b	Phase diagram: Fig. 576. Lattice parameter: Fig. 577.
	5a	Dielectric constant: Fig. 578.
Nr. 1C-b6 $PbTiO_3$-$CaSnO_3$	1b	Phase diagram: see Fig. 576. Lattice parameter: Fig. 579.
	5a	Dielectric constant: Fig. 580.
Nr. 1C-b7 $PbTiO_3$-$SrZrO_3$	1b	Phase diagram: Fig. 581. Lattice parameter: Fig. 582a, b.
	5a	Dielectric constant: Fig. 583.
Nr. 1C-b8 $PbTiO_3$-$SrSnO_3$	1b	Phase diagram: Fig. 584. Lattice parameter: Fig. 585a, b.
	5a	Dielectric constant: Fig. 586.
Nr. 1C-b9 $PbTiO_3$-$BaZrO_3$	1b	Phase diagram: Fig. 587. Lattice parameter: Fig. 588a, b.
	5a	Dielectric constant: Fig. 589.
	7a	Electromechanical property: Tab. 74.

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Tab. 74. $(1-x)PbTiO_3 - xBaZrO_3$ (ceramics). k_p and d_{33} at RT. *[63B15]*

x	Poling field $\cdot 10^5$ V m^{-1} [T in °C]	k_p	d_{33} $\cdot 10^{-12}$ C N^{-1}
0.25	29 [185 ··· 40]	0.16	40
0.30	27 [170 ··· 40]	0.23	50
0.35	39 [145 ··· 40]	0.30	110
0.40	30 [120 ··· 40]	0.17	45

Nr. 1C-b10 $PbTiO_3$-$BaSnO_3$

1b	Phase diagram: Fig. 590. Lattice parameter: Fig. 591a, b.

Nr. 1C-b11 $LaAlO_3$-$BiFeO_3$

1b	Phase diagram: Fig. 592. Lattice parameter: Fig. 593.
5a	Dielectric constant: Fig. 594.

Nr. 1C-b12 $LaCrO_3$-$BiFeO_3$

1b	Phase diagram: Fig. 595. Lattice parameter: Fig. 596a, b.
4	Thermal expansion: Fig. 597.
11	Spontaneous magnetization: see Fig. 595.

Nr. 1C-c1 $NaNbO_3$-$CaTiO_3$

1b	Phase diagram: Fig. 598.
5a	Dielectric constant: Fig. 599.

Nr. 1C-c2 $NaNbO_3$-$BaTiO_3$

1b	Phase diagram: Fig. 600.

Nr. 1C-c3 $NaNbO_3$-$PbTiO_3$

1b	Transition temperature: Fig. 601.
5a	Dielectric constant: Fig. 602.

Nr. 1C-c4 $NaNbO_3$-$PbZrO_3$

1b	Phase diagram: Fig. 603.
5a	Dielectric constant: Fig. 604a, b.

Nr. 1C-c5 $KNbO_3$-$BaTiO_3$

1b	Phase diagram: Fig. 605. Lattice parameter: Fig. 606.
5a	Dielectric constant: Fig. 607a, b, c.

Nr. 1C-c6 $KNbO_3$-$PbTiO_3$

1b	Phase diagram: Fig. 608. Lattice parameter: Fig. 609.
5a	Dielectric constant: Fig. 610a, b.

Nr. 1C-c7 $SrTiO_3$-$BiFeO_3$

1b	Phase diagram: Fig. 611. Lattice parameter: Fig. 612.
5a	Relaxation phenomena are observed in the range II *[65F1]*.

Nr. 1C-c8 $BaTiO_3$-$LaAlO_3$

1b	Lattice parameter and Curie temperature: Tab. 75.

Tab. 75. $BaTiO_3$-$LaAlO_3$. Lattice parameters and Θ_f. [5814]

Concentration mol% BaTiO$_3$	Concentration mol% LaAlO$_3$	a Å	c Å	c/a	V Å^3	Θ_f °C
100.0	—	3.9956	4.0352	1.0100	64.42	+120
99.0	1.0	3.9951	4.0345	1.0098	64.39	+ 87
97.5	2.5	3.9949	4.0293	1.0086	64.30	+ 46
95.0	5.0	4.0050	—	1.0000	64.24	− 14
92.5	7.5	4.0011	—	1.0000	64.05	− 85
90.0	10.0	3.9984	—	1.0000	63.92	−133
87.5	12.5	3.9950	—	1.0000	63.76	—
85.0	15.0	3.9906	—	1.0000	63.55	—
75.0	25.0	3.9800	—	1.0000	63.04	—
—	100.0	3.7950	—	1.000	54.65	—

Nr. 1C-c9 $BaTiO_3$-$BiFeO_3$	11, 12	Néel temperature and magnetic resonance line width: Fig. 613.
Nr. 1C-c10 $PbTiO_3$-$LaAlO_3$	1b	Phase diagram: Fig. 614. Lattice parameter: Fig. 615.
	5a	Dielectric constant: Fig. 616.
Nr. 1C-c11 $PbTiO_3$-$LaMnO_3$	1b	Transition temperatures: Fig. 617. Lattice parameters: Fig. 618.
Nr. 1C-c12 $PbTiO_3$-$LaFeO_3$	1b	Phase diagram: Fig. 619. Lattice parameter: Fig. 620.
	5a	Dielectric constant: Fig. 621.
Nr. 1C-c13 $PbTiO_3$-$BiFeO_3$	1b	Phase diagram: Fig. 622a, b. Lattice parameter: Fig. 623a, b.
	4	Thermal expansion: Fig. 624.
	5a	Dielectric constant: Fig. 625.
Nr. 1C-c14 $PbZrO_3$-$BiFeO_3$	1b	Phase diagram: Fig. 626. Lattice parameter: Fig. 627.
	5a	Dielectric constant: Fig. 628.
Nr. 1C-c15 $SrSnO_3$-$BiFeO_3$	1b	Phase diagram: Fig. 629.
	12c	Mössbauer absorption: Fig. 630.
Nr. 1C-c16 $SrFeO_3$-$BiFeO_3$	1a	Unit cell volume: Fig. 631.
	11	Magnetization: Fig. 632.
Nr. 1C-d1 $SrTiO_3$-$Sr(Fe_{1/2}Ta_{1/2})O_3$	1b	Phase diagram: Fig. 633.
Nr. 1C-d2 $BaTiO_3$-$Ba(Fe_{1/2}Ta_{1/2})O_3$	2b	Phase diagram: Fig. 634.
Nr. 1C-d3 $BaTiO_3$-$(K_{1/2}Bi_{1/2})TiO_3$	1b	Curie temperature: Fig. 635. Lattice parameters: Fig. 636.
Nr. 1C-d4 $PbTiO_3$-$(Na_{1/2}Bi_{1/2})TiO_3$	1b	Phase diagram and lattice parameters: Fig. 637.
	5a	Dielectric constant: Fig. 638.
Nr. 1C-d5 $PbTiO_3$-$(K_{1/2}Bi_{1/2})TiO_3$	1b	Curie temperature and lattice parameters: Fig. 639.
Nr. 1C-d6 $PbTiO_3$-$(Li_{1/2}La_{1/2})TiO_3$	1b	Curie temperature and lattice parameters: Fig. 640.

Nr. 1C-d7 $PbTiO_3$-$(Na_{1/2}La_{1/2})TiO_3$	1b	Curie temperature and lattice parameters: Fig. 641.
Nr. 1C-d8 $PbTiO_3$-$(Li_{1/2}Ce_{1/2})TiO_3$	1b	Lattice parameters: Fig. 642.
Nr. 1C-d9 $PbTiO_3$-$(Li_{1/2}Nd_{1/2})TiO_3$	1b	Lattice parameters: Fig. 643.
Nr. 1C-d10 $PbTiO_3$-$Pb(Mg_{1/2}W_{1/2})O_3$	1b	Phase diagram: Fig. 644. Lattice parameters: Fig. 645.
Nr. 1C-d11 $PbTiO_3$-$Pb(Fe_{1/2}Ta_{1/2})O_3$	1b	Curie temperature: Fig. 646.
Nr. 1C-d12 $PbTiO_3$-$Pb(Sc_{1/2}Nb_{1/2})O_3$	1b	Curie temperature: Fig. 647.
Nr. 1C-d13 $PbTiO_3$-$Pb(Mn_{1/2}Nb_{1/2})O_3$	1b	Transition temperature: Fig. 648. Lattice parameters: Fig. 649.
Nr. 1C-d14 $PbZrO_3$-$Pb(Sc_{1/2}Nb_{1/2})O_3$	1b	Curie temperature: see Fig. 647.
Nr. 1C-d15 $PbZrO_3$-$Pb(Fe_{1/2}Ta_{1/2})O_3$	1b	Curie temperature: Fig. 650.
Nr. 1C-d16 $PbZrO_3$-$(Na_{1/2}Bi_{1/2})ZrO_3$	1b	Phase diagram: Fig. 651.
	4	Lattice distortion: Fig. 652.
	5a	Dielectric constant: Fig. 653.
Nr. 1C-d17 $PbZrO_3$-$(K_{1/2}Bi_{1/2})ZrO_3$	1b	Phase diagram: Fig. 654. Lattice parameters: Tab. 76.
	4	Lattice distortion: Fig. 655.
	5a	Dielectric constants: Fig. 656.

Tab. 76. $(1-x)PbZrO_3 - x(K_{1/2}Bi_{1/2})ZrO_3$. Lattice constants at RT [*62B10*]

x	a Å	b Å	c Å	
0	5.884	11.768	8.220	orthorhombic
0.10	5.882	11.764	8.227	orthorhombic
0.20	5.877	11.755	8.237	orthorhombic
0.30	5.876	11.751	8.248	orthorhombic
0.40	4.151	—	—	cubic
0.50	4.152	—	—	cubic

Nr. 1C-d18 $PbHfO_3$-$Pb(Sc_{1/2}Nb_{1/2})O_3$	1b	Curie temperature: see Fig. 647.
Nr. 1C-d19 $Pb(Mg_{1/2}W_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$	1b	Phase diagram: Fig. 657.
Nr. 1C-d20 $(Na_{1/2}Bi_{1/2})TiO_3$-$(K_{1/2}Bi_{1/2})TiO_3$	1b	Curie temperature: see Fig. 635. Lattice parameters: see Fig. 636.
Nr. 1C-d21 $PbZrO_3$-$(Na_{1/2}Bi_{1/2})TiO_3$	1b	Phase diagram: Fig. 658. Lattice parameters: Fig. 659.
Nr. 1C-d22 $BiFeO_3$-$Sr(Sn_{1/3}Mn_{2/3})O_3$	1b	Phase diagram: Fig. 660. Lattice parameters: Fig. 661.
	12c	Mössbauer effect: see [*65M8*]
Nr. 1C-d23 $BiFeO_3$-$Pb(Fe_{1/2}Nb_{1/2})O_3$	1b	Lattice parameters: Fig. 662.
	5a	Dielectric constant: Fig. 663.
	11	Magnetic susceptibility: Fig. 664. Néel temperature and spontaneous magnetization: Fig. 665.

Nr. 1C-e1 $NaNbO_3$-$LiNbO_3$

1b	Phase diagram: Fig. 666.
5a	Dielectric constant: Fig. 667.

Nr. 1C-e2 $NaNbO_3$-$NaVO_3$

5a	Dielectric constant: Fig. 668.
14b	Switching: see Fig. 9.

Nr. 1C-e3 $NaNbO_3$-$CaNb_2O_6$

1b	Phase diagram: Fig. 669.
5a	Dielectric constant: Fig. 670.

Nr. 1C-e4 $NaNbO_3$-$CdNb_2O_6$

1b	Phase diagram: Fig. 671, 672. Lattice parameter: Fig. 673.
5a	Dielectric constant: Fig. 674; Tab. 77.
7a	Piezoelectricity: Fig. 675; Tab. 78.

Tab. 77. $(1-x)NaNbO_3-(x/2)CdNb_2O_6$ [*56L2*]. r: capacitance ratio; C: Curie constant; Θ_f, Θ compare Fig. 671, 672

Composition x	Firing conditions T °C	t hr	atmosphere	$\varkappa_{RT}$	r	Θ °C	$\varkappa_{max}$	Θ_f °C	C $\cdot 10^4$ °C	Θ_p °C	ϱ 10^3 kg m^{-3}
0.02	1250	1	CdO	230	—	200	2700	375	12	345	3.9
0.05	1250	1	CdO	500	1200	60	4000	375	12	345	4.2
0.10	1250	1	CdO	1000	130	75	4100	320	18	275	4.3
0.15	1250	1	CdO	1400	40	50	8500	285	24	260	4.3
0.20	1250	1	CdO	2300	20	20	10000	250	14	250	4.4
0.25	1250	1	CdO	3500	10	5	15000	220	20	230	4.5
0.30	1220	2	CdO	2700	12	−25	11000	210	20	205	4.6

Tab. 78. $(1-x)NaNbO_3-(x/2)CdNb_2O_6$ (ceramics) [*62K4*]

x	0.05	0.10	0.15	0.20	0.25	0.30	
ϱ	4.2	4.3	4.3	4.3	4.4	4.2	10^3 kg m^{-3}
$f_R \cdot 2r$	3.0	3.0	3.0	3.15	3.36	3.25	10^3 Hz m
s_{11}^E	11.9	11.6	11.6	10.5	9.0	10.1	10^{-12} m^2 N^{-1}
tan δ	0.01	0.01	0.02	0.01	0.01	0.03	
$\varkappa$ at Θ_f	4	4.1	8.5	16	13	11	10^3

Nr. 1C-e5 $NaNbO_3$-$SrNb_2O_6$

1b	Phase diagram: Fig. 676. Lattice parameter: Fig. 677.
5a	Dielectric constant: Fig. 678.
7a	Electromechanical properties: Fig. 679, 680, 681.

Nr. 1C-e6 $NaNbO_3$-$PbNb_2O_6$

1b	Phase diagram: Fig. 682. Lattice parameter: Fig. 683.
7a	Electromechanical properties: Fig. 684.

Nr. 1C-e7 $CdTiO_3$-$LiNbO_3$, $CdTiO_3$-$LiTaO_3$

5a	Dielectric constant: Fig. 685.

Nr. 1C-e8 $SrTiO_3$-$Bi_2O_3 \cdot 3TiO_2$

1b	Lattice parameter: Fig. 686.
5a	Dielectric constant: Fig. 687, 688.

Nr. 1C-e9 $BaTiO_3$-$BaNb_2O_6$

1b	Phase diagram: Fig. 689.

Nr. 1C-e10 $BaTiO_3$-$BaTa_2O_6$	1b	Lattice parameter: Fig. 690.
	5a	Dielectric constant: Fig. 691.
Nr. 1C-e11 $BaTiO_3$-$A_2B_2O_7$	1b	Curie temperature: Fig. 692.
	5a	Dielectric constant: Fig. 693 ··· 697.

Nr. 1C-e12 $PbZrO_3$-$PbNb_2O_6$

For the solid solution with $PbNb_2O_6$ as an end material see 5B-8.

	1b	Phase diagram: Fig. 698.
	4	Thermal expansion: Fig. 699.
	5	Dielectric constant: Fig. 700.
Nr. 1C-e13 $PbZrO_3$-$PbTa_2O_6$	1b	Phase diagram: Fig. 701.
	4	Thermal expansion: see Fig. 699.
	5	Dielectric constant: Fig. 702.
Nr. 1C-f1 $CaTiO_3$-$SrTiO_3$-$BaTiO_3$	1b	Phase diagram: Fig. 703.
Nr. 1C-f2 $CaTiO_3$-$BaTiO_3$-$PbTiO_3$	1b	Phase diagram: Fig. 704, 705. Curie temperature: Fig. 706.
	7a	Electromechanical properties: see Nr. 1A-8, 7a.
Nr. 1C-f3 $PbTiO_3$-$PbZrO_3$-$PbO:SnO_2$	1b	Phase diagram: Fig. 707.
	8b	Elastic properties: Fig. 708, 709.
Nr. 1C-f4 $PbTiO_3$-$PbHfO_3$-$PbO:SnO_2$	1b	Phase diagram: Fig. 710.
Nr. 1C-f5 $PbTiO_3$-$PbZrO_3$-$LaFeO_3$	1b	Phase diagram: Fig. 711. Lattice parameters: Fig. 712.
Nr. 1C-f6 $PbTiO_3$-$PbZrO_3$-$BiFeO_3$	1b	Phase diagram: Fig. 713. Lattice parameters: Fig. 714.
Nr. 1C-f7 $PbTiO_3$-$PbZrO_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$	1b	Phase diagram: Fig. 715. Lattice parameters: Fig. 716.
	7a	Electromechanical property: Fig. 717, 718.
Nr. 1C-f8 $PbTiO_3$-$PbZrO_3$-$Pb(Fe_{1/2}Nb_{1/2})O_3$	1b	Lattice parameters: Fig. 719. Curie temperature: Fig. 720.
	7a	Electromechanical property: Fig. 721.
Nr. 1C-f9 $PbTiO_3$-$PbZrO_3$-ABO_3	1b	Phase diagram: Fig. 722.
Nr. 1C-f10 $PbTiO_3$-$SrTiO_3$-$LaMnO_3$	1b	Curie temperature: Fig. 723.

Nr. 1C-f11 $PbTiO_3$-$LaMnO_3$-$LaMeO_3$ (Me = Fe, Co, Ni, Cr)

	1b	Transition temperatures: Fig. 724.
	5a	Dielectric constant: Fig. 725.
	11	Magnetic susceptibility: see Fig. 725. Magnetization: Fig. 726.

Nr. 1C-f12 $BaTiO_3$-$SrTiO_3$-$LaYO_3$-$LaInO_3$	1b	Phase diagram: Fig. 727.
Nr. 1C-f13 $CaSnO_3$-$SrSnO_3$-$BaSnO_3$	1b	Phase diagram: Fig. 728.
Nr. 1C-f14 (Na-K)(Nb-Ta)O_3	1b	Phase diagram: Fig. 729.
Nr. 1C-f15 (Ca-Ba)(Ti-Zr)O_3	1b	Phase diagram: Fig. 730.
Nr. 1C-f16 (Sr-Pb)(Ti-Zr)O_3	1b	Phase diagram: Fig. 731. Lattice parameter: Fig. 732. Transition temperature: Fig. 733.
	5a	Dielectric constant: Fig. 734, 735.
Nr. 1C-f17 (Ba-Pb)(Ti-Zr)O_3	1b	Phase diagram: Fig. 736. Lattice parameter: Fig. 737. Transition temperature: Fig. 738.
	7a	Electromechanical properties: Fig. 739, 740.
Nr. 1C-f18 (Ba-Pb)(Ti-Sn)O_3	1b	Phase diagram: Fig. 741, 742. Lattice parameter: Fig. 743. Transition temperature: Fig. 744.
Nr. 1C-f19 $BaTiO_3$-$PbTiO_3$-$BaNb_2O_6$-$PbNb_2O_6$	1b	Phase diagram: Fig. 745. Lattice parameter: Fig. 746.

2 WO_3

2A Pure compound

Nr. 2A-1 WO_3, Tungsten trioxide

1a The anomalous dielectric properties of ceramic specimens of WO_3 were discovered by OGAWA[a]) in 1948. Possibility of ferroelectricity in WO_3 was pointed out by MATTHIAS[b]) in 1949. — [a])*48N1, 48N2* [b])*49M2*

b

phase	VII	VI	V	IV	III	II	I	
state	F[a])							[a])*49M2*
crystal system	mono-clinic*[b])	tri-clinic[b])	mono-clinic[c])	ortho-rhombic[b])	tetra-gonal[d])	tetra-gonal[b])	tetra-gonal[b])	[b])*60T1* [c])*60T2*
space group			$P2_1/n$[c]) $-C^5_{2h}$		$P4/nmm$[d]) $-D^7_{4h}$			[d])*52K1*
Θ		−40[b])	17[b])	330[e])	740[e])	910[e])	1230[e]) °C	[e])*56S1*

$T_{melt} = 1473$ °C. — *21J1*
$\varrho = 7.157 \cdot 10^3$ kg m^{-3} at RT. — *04S1*
$a = 7.30$ Å, $b = 7.53$ Å, $c = 7.68$ Å, $\beta = 90° 54'$ at 30 °C. — *60T1*
Transparent, bluish green.

2a Crystal growth: Sublimation method. — *51U1, 56T2, 59S3*

b Crystal form: Plate-like.

3 Crystal structure: Fig. 747, 748; Tab. 79; Fig. 749.

phase	VII	VI	V	IV	III	II	I
Z	4	8	8				

— *60T1*

4 Lattice distortion: Tab. 80.
Thermal expansion: Fig. 750 ··· 754.

5a Dielectric constant: $\varkappa = 100 \cdots 300$ at liquid air temperature. — *49M2*
No reliable dielectric measurements could be carried out at and above room temperature because of high electrical conductivity.
$d\Theta_{IV-III}/dp = -8.46 \cdot 10^{-8}$ °K N^{-1} m^2. — *66T4*

c Dielectric hysteresis loop was observed at liquid air temperature. — *49M2*

* As to the crystal system in the phase VII, possibility of triclinic symmetry was discussed by TANISAKI [*60T1*].

V Index of substances — Substanzenverzeichnis

This index consists of two parts: part A is for pure compounds (including complex compounds such as $Pb(Co_{1/2}Nb_{1/2})O_3$ or $Na_{0.5}Bi_{4.5}Ti_4O_{15}$) and part B is for solid solutions.

V A: In the 1st column the substances are ordered according to the alphabetically arranged gross formula. When their names (e.g. Rochelle salt) and/or their abbreviated names (e.g. TGS) are widely used, they are also included in this column. In the gross formula the numbers of the elements are determined by simple addition.

Compounds containing water of crystallization are, however, listed twice: (1) H and O of the water molecules are included in the gross formula, (2) the water molecules are attached separately to the gross formula. For instance, Rochelle salt is listed in the 1st column as $\mathbf{C}_4H_4KNaO_6 \cdot 4H_2O$, $\mathbf{C}_4H_{12}KNaO_{10}$ and also as **R**ochelle salt, **R**S, **S**eignette salt.

Crystals in which H is replaced by D (e.g. KD_2PO_4) are not listed separately, since data on their properties are presented in the same section as the data on the non-deuterated crystals (e.g. KH_2PO_4).

V B: In the 1st column the gross formula of each end material of a solid solution (e.g. $BaTiO_3$ or $PbTiO_3$ for the solid solution $BaTiO_3$–$PbTiO_3$) is listed in the same manner as in the case of pure compounds. Thus the solid solution $BaTiO_3$–$PbTiO_3$ can be found in the 2nd column by looking first for either BaO_3Ti or O_3PbTi in the 1st column of Part B. If the solid solution is expressed by the formula such as $(Sb_xBi_{1-x})SI$, the end material can be obtained by putting x equal to either 0 or 1. When solid solutions have abbreviated names (e.g. KTN), these are also included in the 1st column.

Since in general one section corresponds to one substance in this volume, the 3rd column gives the section number and the 4th column gives the first page of the section.

Dieses Verzeichnis besteht aus zwei Teilen: Teil A enthält die reinen Verbindungen (einschließlich komplexer Verbindungen wie $Pb(Co_{1/2}Nb_{1/2})O_3$ oder $Na_{0.5}Bi_{4.5}Ti_4O_{15}$) und Teil B enthält die Mischkristalle.

V A: In der 1. Spalte sind die Substanzen nach der alphabetisch angeordneten Bruttoformel aufgeführt. Wenn ihre Namen (z. B. Seignette-Salz) und/oder ihre abgekürzten Bezeichnungen (z. B. TGS) häufig gebraucht werden, sind auch sie in dieser Spalte zu finden. In der Bruttoformel ist die Anzahl jedes Elements durch einfache Addition bestimmt.

Verbindungen, die Kristallwasser enthalten, sind zweimal aufgeführt: 1. H und O der Wassermoleküle sind in der Bruttoformel enthalten. 2. die Wassermoleküle werden getrennt der Bruttoformel hinzugefügt (z. B. Seignette-Salz ist in der 1. Spalte aufgeführt als $\mathbf{C}_4H_4KNaO_6 \cdot 4H_2O$, $\mathbf{C}_4H_{12}KNaO_{10}$ und auch als **R**ochelle-Salz, **R**S, **S**eignette-Salz).

Kristalle, in denen H durch D ersetzt ist (z. B. KD_2PO_4), werden nicht gesondert aufgeführt. Daten von ihren Eigenschaften erscheinen in demselben Abschnitt an der gleichen Stelle wie die Daten von den nicht deuterierten Kristallen (z.B. KH_2PO_4).

V B: In der 1. Spalte ist die Bruttoformel jeder Endsubstanz einer Mischkristallreihe (z. B. $BaTiO_3$ oder $PbTiO_3$ für die Mischkristallreihe $BaTiO_3$–$PbTiO_3$) in derselben Weise aufgeführt wie im Fall von reinen Verbindungen. So kann die Mischkristallreihe $BaTiO_3$–$PbTiO_3$ in der zweiten Spalte gefunden werden, wenn man zunächst entweder BaO_3Ti oder O_3PbTi in der ersten Spalte von Teil B sucht. Wenn die Mischkristallreihe durch die Formel $(Sb_xBi_{1-x})SI$ ausgedrückt wird, kann man die Endsubstanz finden, indem man x gleich 0 oder 1 setzt. Wenn Mischkristalle abgekürzte Namen haben (z. B. KTN), sind diese auch in der 1. Spalte enthalten.

Da in diesem Band jeweils ein Abschnitt einer Substanz entspricht, gibt die 3. Spalte die Abschnittsnummer und die 4. Spalte die erste Seite des Abschnitts an.

VA Pure compounds

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VB Solid solutions

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Gross formula	Chemical formula	Nr.	Page
O_3PbTi	$PbTiO_3$–$NaNbO_3$	1C–c3	83
O_3PbTi	$PbTiO_3$–$Pb(Fe_{1/2}Ta_{1/2})O_3$	1C–d11	85
O_3PbTi	$PbTiO_3$–$PbHfO_3$	1C–a29	82
O_3PbTi	$PbTiO_3$–$Pb(Mg_{1/2}W_{1/2})O_3$	1C–d10	85
O_3PbTi	$PbTiO_3$–$Pb(Mn_{1/3}Nb_{1/2})O_3$	1C–d13	85
O_3PbTi	$PbTiO_3$–$PbNb_2O_6$	5B–7	101
O_3PbTi	$PbTiO_3$–$PbO:SnO_2$	1C–a30	82
O_3PbTi	$PbTiO_3$–$Pb(Sc_{1/2}Nb_{1/2})O_3$	1C–d12	85
O_3PbTi	$PbTiO_3$–$PbZrO_3$	1C–a27	77
O_3PbTi	$PbTiO_3$–$SrSnO_3$	1C–b8	82
O_3PbTi	$PbTiO_3$–$SrTiO_3$	1C–a10	75
O_3PbTi	$PbTiO_3$–$SrZrO_3$	1C–b7	82
O_3PbTi	$PbTiO_3$–ABO_3–$PbZrO_3$	1C–f9	87
O_3PbTi	$PbTiO_3$–$BaTiO_3$–$CaTiO_3$	1C–f2	87
O_3PbTi	$PbTiO_3$–$BiFeO_3$–$PbZrO_3$	1C–f6	87
O_3PbTi	$PbTiO_3$–$LaCoO_3$–$LaMnO_3$	1C–f11	87
O_3PbTi	$PbTiO_3$–$LaCrO_3$–$LaMnO_3$	1C–f11	87
O_3PbTi	$PbTiO_3$–$LaFeO_3$–$LaMnO_3$	1C–f11	87
O_3PbTi	$PbTiO_3$–$LaFeO_3$–$PbZrO_3$	1C–f5	87
O_3PbTi	$PbTiO_3$–$LaMnO_3$–$LaNiO_3$	1C–f11	87
O_3PbTi	$PbTiO_3$–$LaMnO_3$–$SrTiO_3$	1C–f10	87
O_3PbTi	$PbTiO_3$–$Pb(Fe_{1/2}Nb_{1/2})O_3$–$PbZrO_3$	1C–f8	87
O_3PbTi	$PbTiO_3$–$PbHfO_3$–$PbO:SnO_2$	1C–f4	87
O_3PbTi	$PbTiO_3$–$Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbZrO_3$	1C–f7	87
O_3PbTi	$PbTiO_3$–$PbO:SnO_2$–$PbZrO_3$	1C–f3	87
O_3PbTi	$PbTiO_3$–$BaTiO_3$–$BaNb_2O_6$–$PbNb_2O_6$	1C–f19	88
O_3PbTi	(Pb–Ba)(Ti–Sn)O_3	1C–f18	88
O_3PbTi	(Pb–Ba)(Ti–Zr)O_3	1C–f17	88
O_3PbTi	Pb(Ti–Zr)O_3	1C–a28	78
O_3PbTi	(Pb–Sr)(Ti–Zr)O_3	1C–f16	88
O_3PbZr	$PbZrO_3$–$BaTiO_3$	1C–b3	82
O_3PbZr	$PbZrO_3$–$BaZrO_3$	1C–a15	76
O_3PbZr	$PbZrO_3$–$BiFeO_3$	1C–c14	84
O_3PbZr	$PbZrO_3$–$CaZrO_3$	1C–a13	76
O_3PbZr	$PbZrO_3$–$(K_{1/2}Bi_{1/2})ZrO_3$	1C–d17	85
O_3PbZr	$PbZrO_3$–$(Na_{1/2}Bi_{1/2})TiO_3$	1C–d21	85
O_3PbZr	$PbZrO_3$–$(Na_{1/2}Bi_{1/2})ZrO_3$	1C–d16	85
O_3PbZr	$PbZrO_3$–$NaNbO_3$	1C–c4	83
O_3PbZr	$PbZrO_3$–$Pb(Fe_{1/2}Ta_{1/2})O_3$	1C–d15	85
O_3PbZr	$PbZrO_3$–$PbHfO_3$	1C–a31	82
O_3PbZr	$PbZrO_3$–$PbNb_2O_6$	5B–8, 1C–e12	101, 87
O_3PbZr	$PbZrO_3$–$PbO:SnO_2$	1C–a32	82
O_3PbZr	$PbZrO_3$–$Pb(Sc_{1/2}Nb_{1/2})O_3$	1C–d14	85
O_3PbZr	$PbZrO_3$–$PbTa_2O_6$	1C–e13	87
O_3PbZr	$PbZrO_3$–$PbTiO_3$	1C–a27	77
O_3PbZr	$PbZrO_3$–$SrZrO_3$	1C–a14	76
O_3PbZr	Pb(Zr–Ti)O_3 (PZT)	1C–a28	78
O_3PbZr	$PbZrO_3$–ABO_3–$PbTiO_3$	1C–f9	87
O_3PbZr	$PbZrO_3$–$BiFeO_3$–$PbTiO_3$	1C–f6	87
O_3PbZr	$PbZrO_3$–$LaFeO_3$–$PbTiO_3$	1C–f5	87
O_3PbZr	$PbZrO_3$–$Pb(Fe_{1/2}Nb_{1/2})O_3$–$PbTiO_3$	1C–f8	87
O_3PbZr	$PbZrO_3$–$Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbTiO_3$	1C–f7	87
O_3PbZr	$PbZrO_3$–$PbO:SnO_2$–$PbTiO_3$	1C–f3	87
O_3PbZr	(Pb–Ba)(Zr–Ti)O_3	1C–f17	88
O_3PbZr	(Pb–Sr)(Zr–Ti)O_3	1C–f16	88
O_3SnSr	$SrSnO_3$–$BaSnO_3$	1C–a20	76
O_3SnSr	$SrSnO_3$–$BiFeO_3$	1C–c15	84
O_3SnSr	$SrSnO_3$–$CaSnO_3$	1C–a19	76
O_3SnSr	$SrSnO_3$–$PbTiO_3$	1C–b8	82
O_3SnSr	$SrSnO_3$–$BaSnO_3$–$CaSnO_3$	1C–f13	88
O_6SrTa_2	$SrTa_2O_6$–$PbTa_2O_6$	5B–16	102
O_6SrTa_2	(Sr–Ba–Pb)(Ta–Nb)$_2O_6$	5B–15	102
$O_7Sr_2Ta_2$	$Sr_2Ta_2O_7$–$Ca_2Ta_2O_7$	6B–6	106

Gross formula	Chemical formula	Nr.	Page
$O_7Sr_2Ta_2$	$Sr_2Ta_2O_7$–$Sr_2Nb_2O_7$	6B–5	106
O_3SrTi	$SrTiO_3$–$BaTiO_3$	1C–a9	75
O_3SrTi	$SrTiO_3$–$BiFeO_3$	1C–c7	83
O_3SrTi	$SrTiO_3$–$Bi_2O_3 \cdot 3TiO_2$	1C–e8	86
O_3SrTi	$SrTiO_3$–$CaTiO_3$	1C–a6	74
O_3SrTi	$SrTiO_3$–$PbTiO_3$	1C–a10	75
O_3SrTi	$SrTiO_3$–$Sr(Fe_{1/2}Ta_{1/2})O_3$	1C–d1	84
O_3SrTi	$SrTiO_3$–$BaTiO_3$–$CaTiO_3$	1C–f1	87
O_3SrTi	$SrTiO_3$–$LaMnO_3$–$PbTiO_3$	1C–f10	87
O_3SrTi	$SrTiO_3$–$BaTiO_3$–$LaInO_3$–$LaYO_3$	1C–f12	88
O_3SrTi	$(Sr$–$Pb)(Ti$–$Zr)O_3$	1C–f16	88
O_3SrZr	$SrZrO_3$–$PbTiO_3$	1C–b7	82
O_3SrZr	$SrZrO_3$–$PbZrO_3$	1C–a14	76
O_3SrZr	$(Sr$–$Pb)(Zr$–$Ti)O_3$	1C–f16	88
PZT	$Pb(Zr$–$Ti)O_3$	1C–a28	78
SnTe	SnTe–GeTe	36–3	214